Elektrificatie van de Industrie: Power to Chemicals

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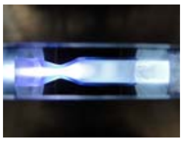
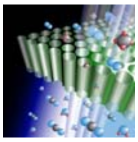
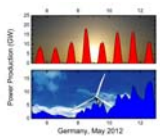
EINDHOVEN, THE NETHERLANDS

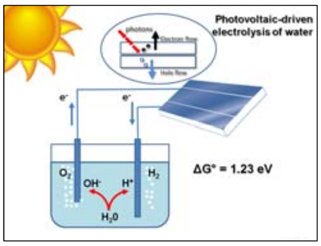




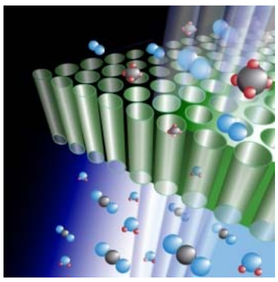
NNV Energie & Klimaat 9 juni 2017

DIFFER is part of NWO

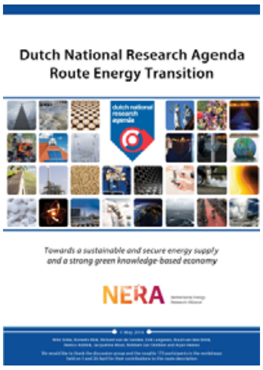
Contents

- **The Energy Transition**
  - Greening the (chemical) industry
  - Electricity to fuels, feedstock
- **P2G;P2L;P2X; (P2Heat)**
- **Summary**





The energy transition:
the route towards the energy infrastructure in 2050



Towards a sustainable and secure energy supply and a strong green knowledge-based economy

- 10 Research challenges defined to reach a CO_2 neutral energy infrastructure;
- Research challenges cross-cutting all sciences

- 4 Functionalities of energy:
  - Low temperature heat
  - High temperature heat
  - Transport & mobility
  - Light and devices

http://www.nera.nl/wp-content/uploads/2016/08/Dutch-National-Research-Agenda-Route-Energy-Transition.pdf

The energy transition:
the route towards the energy infrastructure in 2050

A CO_2-neutral energy society will be different

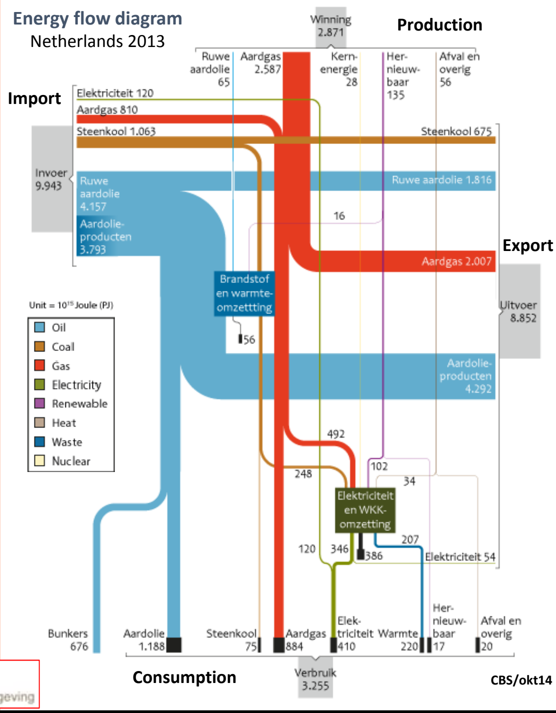
A CO_2-neutral energy system will probably look very different from our current fossil fuel-based society. It is very important to properly understand the changes that will take place due to the transition to a CO_2-neutral energy society. Insight into the societal changes within and beyond the energy sector is important to be able to manage the transition process and to adjust it where necessary. Elements of this transition include a different spatial design, a transition to circular processes, new forms of transport, infrastructure for energy carriers (electricity, hydrogen, etc.) and changing lifestyles. Public acceptance of certain solutions will also determine the resulting transition process and societal structure.

nationale wetenschapsagenda: 19 25 38 40 70 108

Fossil fuels determines how our society is organized

- Consumer vs. prosumer; central vs. decentral
- Circular economy is needed
- New forms of transport
- Public acceptance is crucial and determines pace
- ....

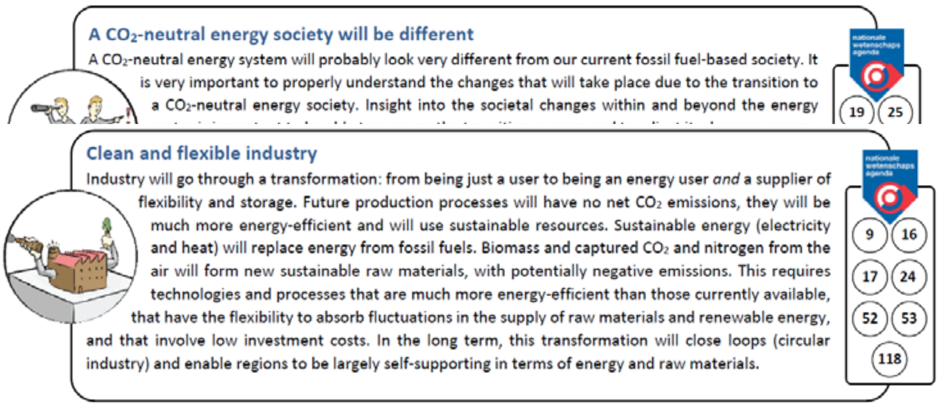
http://www.nera.nl/wp-content/uploads/2016/08/Dutch-National-Research-Agenda-Route-Energy-Transition.pdf



Compendium voor de Leefomgeving

- **Energy flow diagram Netherlands (2013)**
- **Energy use in society**
  - Fuels: 67%
  - Electricity: 13%
  - Heat: 20%

The energy transition:
the route towards the energy infrastructure in 2050



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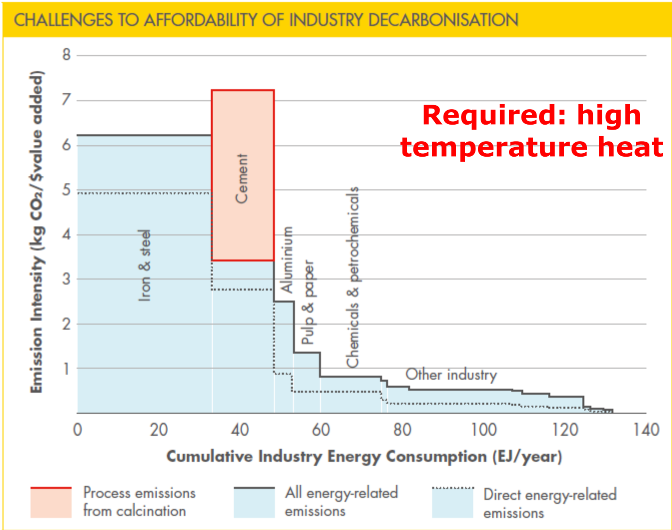
Clean and flexible industry

Industry will go through a transformation: from being just a user to being an energy user *and* a supplier of flexibility and storage. Future production processes will have no net CO_2 emissions, they will be much more energy-efficient and will use sustainable resources. Sustainable energy (electricity and heat) will replace energy from fossil fuels. Biomass and captured CO_2 and nitrogen from the air will form new sustainable raw materials, with potentially negative emissions. This requires technologies and processes that are much more energy-efficient than those currently available, that have the flexibility to absorb fluctuations in the supply of raw materials and renewable energy, and that involve low investment costs. In the long term, this transformation will close loops (circular industry) and enable regions to be largely self-supporting in terms of energy and raw materials.

Greening the (chemical) industry, high temperature heat, feedstock (carbon, hydrogen, nitrogen, biomass, …..

http://www.nera.nl/wp-content/uploads/2016/08/Dutch-National-Research-Agenda-Route-Energy-Transition.pdf

Greening the industry

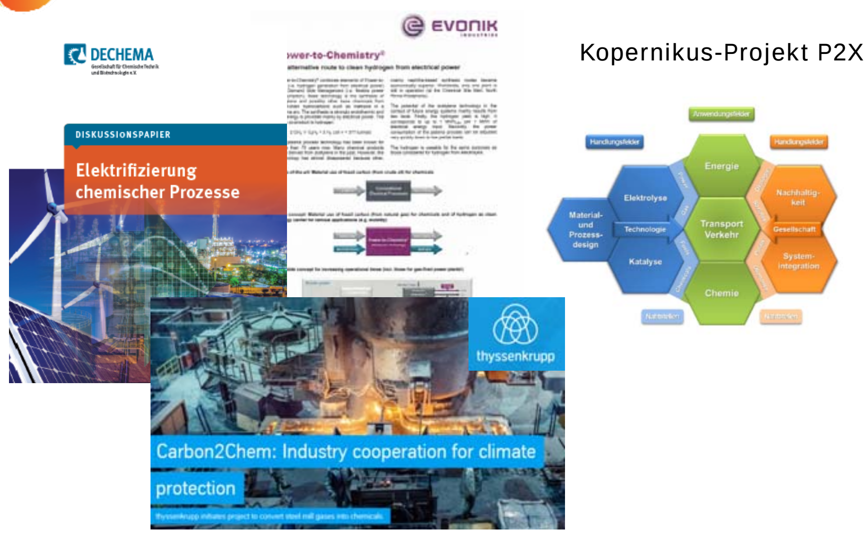


Source: Shell analysis based on data from IEA and Oxford Economics.

Shell report *A better life with a healthy planet (2016)*

Electrification of the chemical industry

Kopernikus-Projekt P2X



Electrochemistry key technology; examples not yet circular!!

The energy transition:
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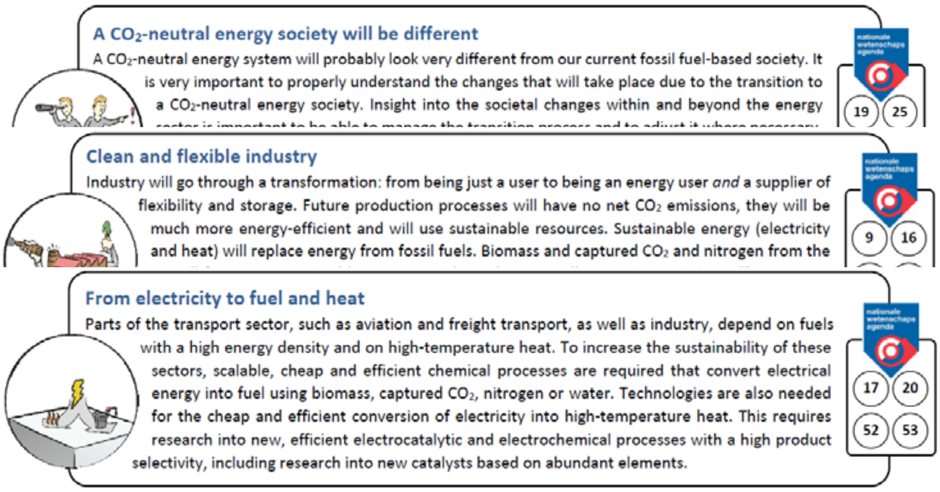

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19 25

Clean and flexible industry

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9 16

From electricity to fuel and heat

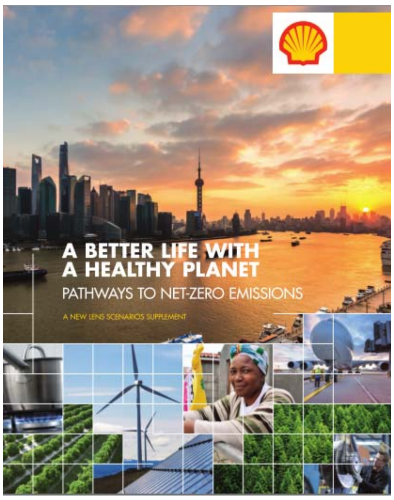
Parts of the transport sector, such as aviation and freight transport, as well as industry, depend on fuels with a high energy density and on high-temperature heat. To increase the sustainability of these sectors, scalable, cheap and efficient chemical processes are required that convert electrical energy into fuel using biomass, captured CO_2, nitrogen or water. Technologies are also needed for the cheap and efficient conversion of electricity into high-temperature heat. This requires research into new, efficient electrocatalytic and electrochemical processes with a high product selectivity, including research into new catalysts based on abundant elements.

17 20 52 53

From electricity to fuels and heat

http://www.nera.nl/wp-content/uploads/2016/08/Dutch-National-Research-Agenda-Route-Energy-Transition.pdf

The energy transition:
The energy infrastructure in 2050

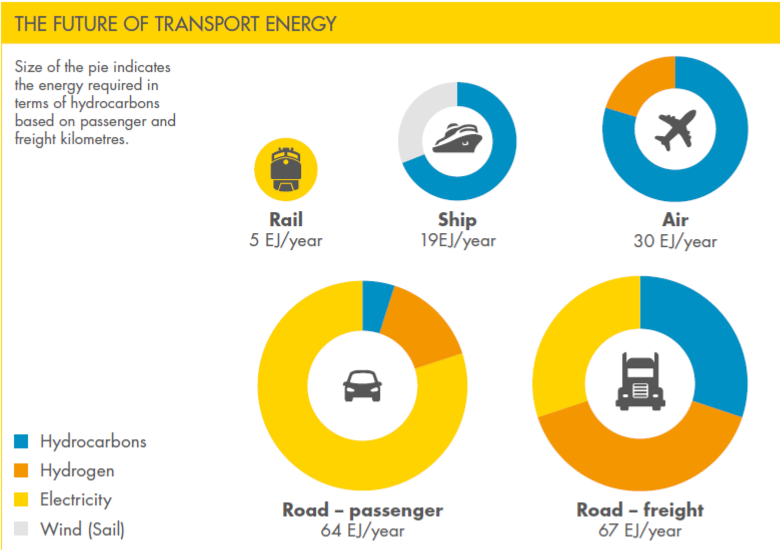


Many references to abundancy of renewable electricity and surplus electrons.......

"However, the real milestone is reached when an offshore hydrogen electrolysis system is built utilising the growing surplus ***electrons*** *from those wind farms…."*

http://www.nera.nl/wp-content/uploads/2016/08/Dutch-National-Research-Agenda-Route-Energy-Transition.pdf

Future of transport energy



Shell report *A better life with a healthy planet (2016)*

Electricity to high energy density fuels

FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT

arpa·e

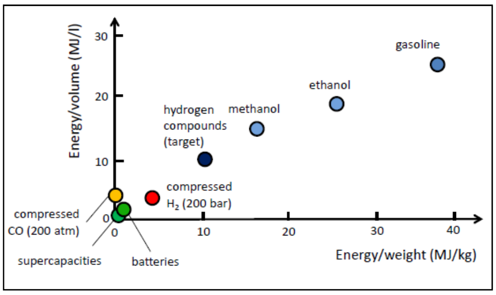
ADVANCED RESEARCH PROJECTS AGENCY – ENERGY (ARPA-E)
U.S. DEPARTMENT OF ENERGY

RENEWABLE ENERGY TO FUELS THROUGH UTILIZATION OF ENERGY-DENSE LIQUIDS (REFUEL)

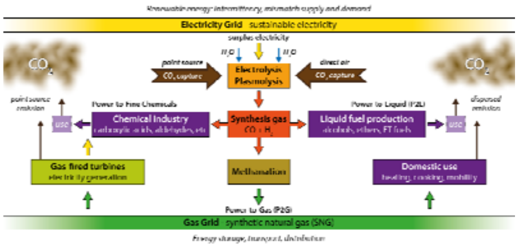
Announcement Type: Initial Announcement
Funding Opportunity No. DE-FOA-0001562
CFDA Number 81.135

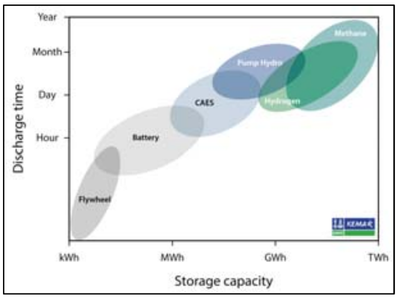
ARPA-E is sollicitng proposals on (renewable) electricity to energy-dense liquid (fuels)

Think about liquid hydrocarbons, NH_3,….



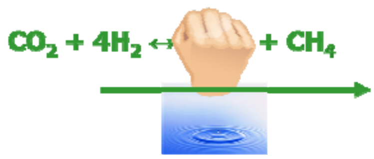
Why would hydro-carbons be a good choice?

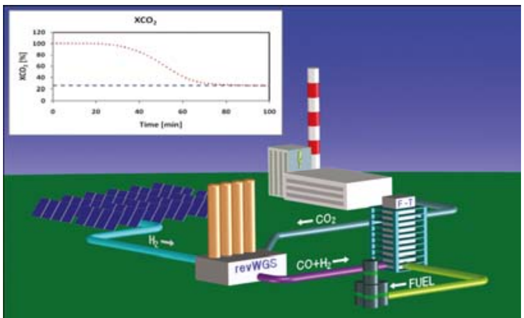




- Ideal for energy storage
  - High energy density per volume and per mass
- Use of existing hydro-carbon infrastructure
  - Transport, distribution and use
- Coupling electricity and gas system: Power-to-Gas (P2G)
  - Large storage capacity in gas grid (surplus RE electricity)
  - NL gas grid ~ 552 TWh (one day EU electrical power ~ 10 TWh)

Artist impression P2Fuel (using sorption enhanced methanation)



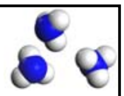


Haije & Geerlings dx.doi.org/10.1021/es203160k

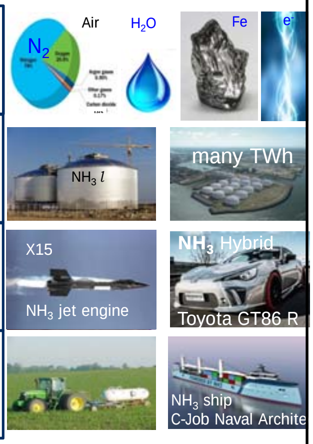
TUDelft Courtesy of W. Haije (TUD) Challenge the future

Ammonia

Ammonia NH_3 for large scale energy storage



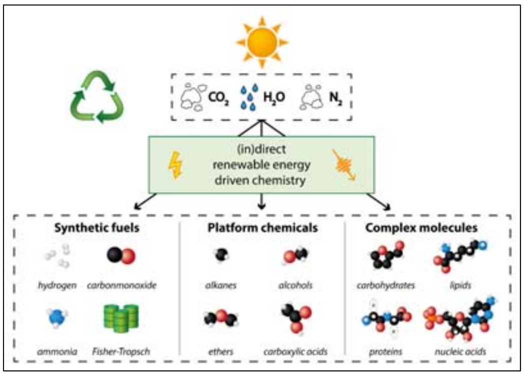
Production	➢ based on abundant elements N, H, and cheap catalysts: scalable. ➢ can be produced using abundant renewable electricity and CO_2 free.
Storage	➢ energy density NH_3: 22.5 MJ/kg (HHV) ➢ liquid at 10 Bar, 20 °C ➢ current containers can contain 60000 ton NH_3~ 375 GWh.
Use	➢ potentially clean use in fuel cell, combustion engine, gas turbine. No CO_2. ➢ fertilizer industry: CO_2 neutral fertilizers
Acceptance	➢ poisonous, but 100⁺ yr industrial know-how ➢ current NH_3 production costs >1.5% of world energy use >6 EJ/yr ➢ Bio degradable (fertilizer)



TUDelft

Courtesy of F. Mulder (TUD)

CO_2 neutral fuels, P2X, P2G, P2L

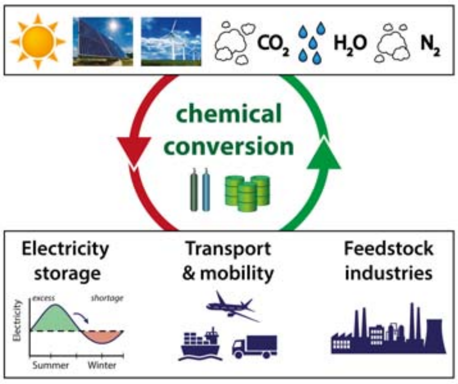


- Excellent potential to harness solar energy
- Enables storage of sustainable energy in CO_2-neutral chemical fuels
- Essential ingredient in the future sustainable energy infrastructure
- Essential to provide future carbon based chemical feedstock!

P2X, P2L, P2G: research and technology

Direct (light) & **indirect** (electricity) technologies

Point source & **direct air capture**
- purity and scale
- CCS → CCU



Conversion:
- efficiency
- scalability
- products
- processes

Footprint?
- life cycle assessments
- environment

Role for fundamental and applied research
- new materials, from separation membranes to catalysts,
- exploiting disruptive processes & incrementally improving state-of-the-art

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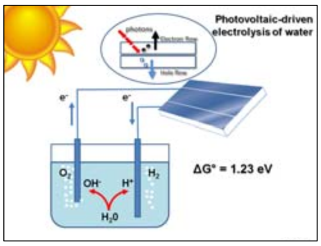
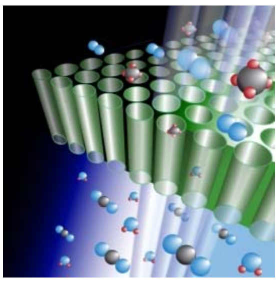


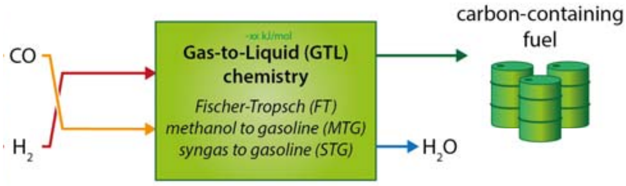


Production of synthetic fuels (hydrocarbons)

Fischer-Tropsch process

FT hier als voorbeeld maar equivalent proces (Haber-Bosch) voor ammonia productie vanuit H_2 en N_2

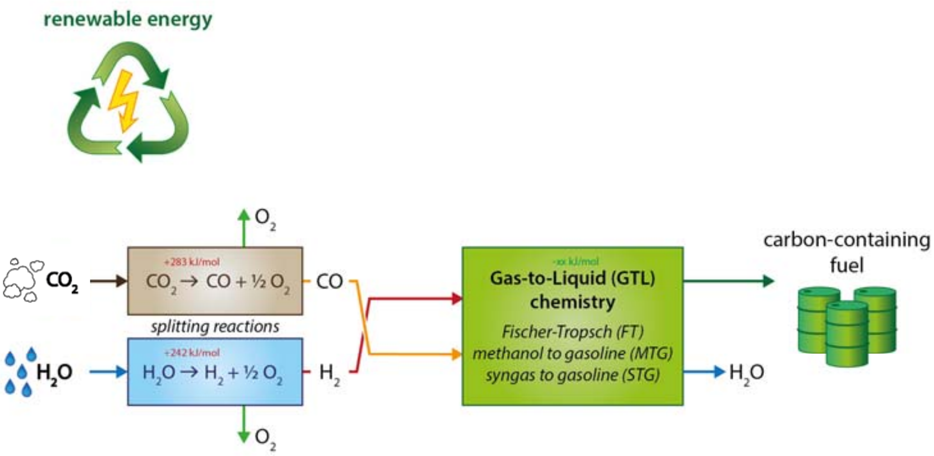
Syngas (H2/CO)



Syngas produced from steam reformation of methane gas (< €/kg)

reaction enthalpies calculated for gaseous products at standard conditions

Full chain of CO_2 neutral fuels



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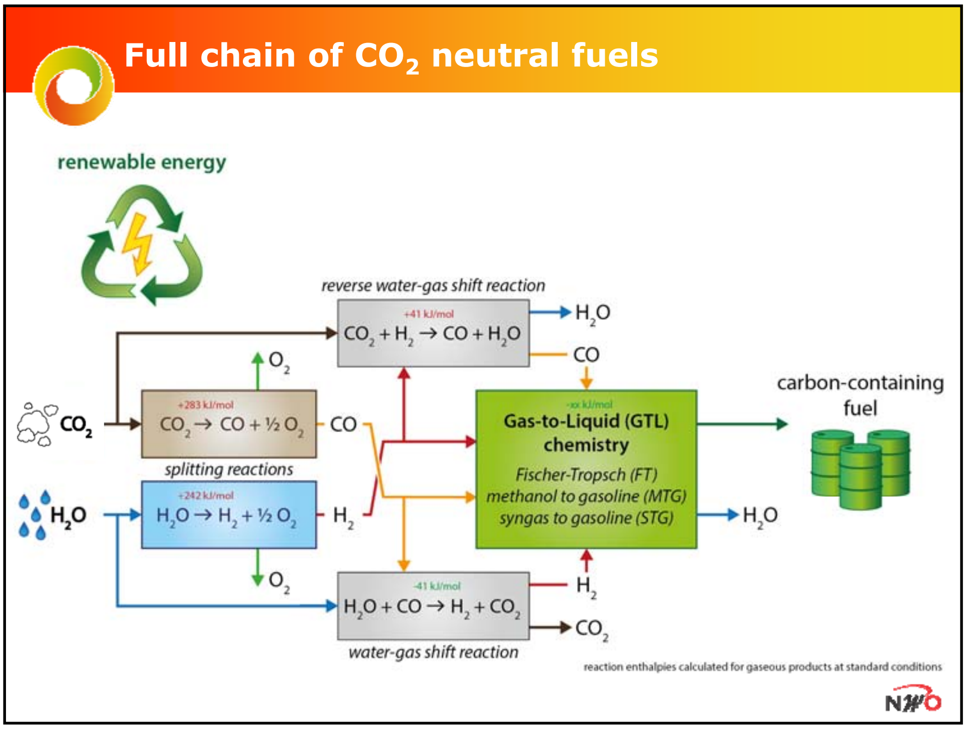
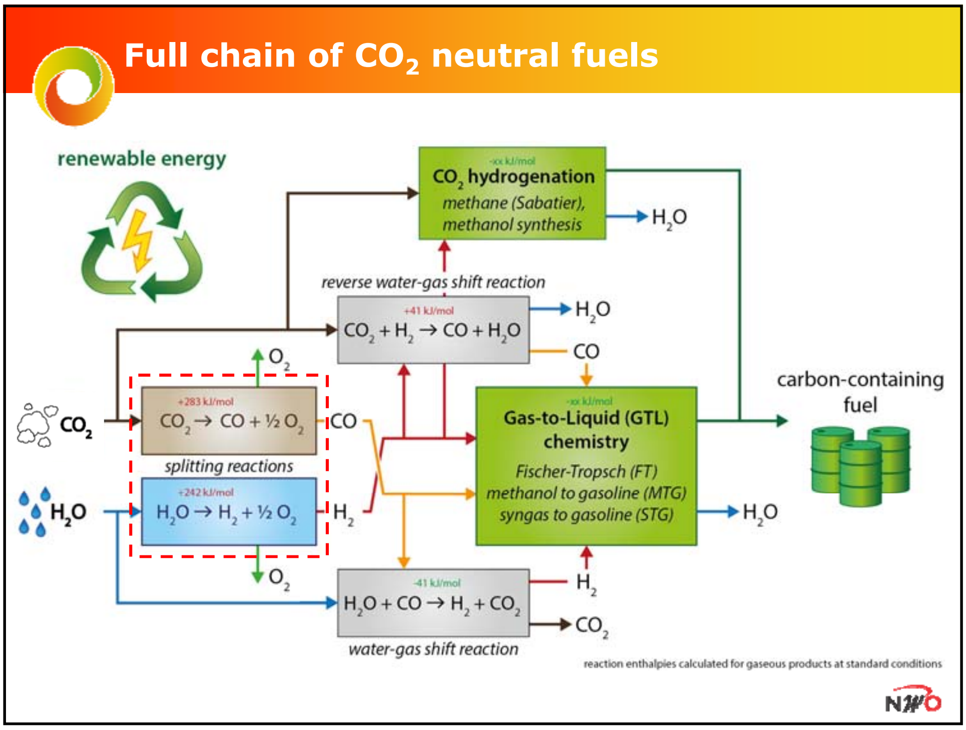


Full chain of CO_2 neutral fuels
renewable energy
reverse water-gas shift reaction
+41 kJ/mol
$CO_2 + H_2 \rightarrow CO + H_2O$
H_2O
CO
O_2
CO_2
+283 kJ/mol
$CO_2 \rightarrow CO + ½ O_2$
CO
splitting reactions
+242 kJ/mol
$H_2O \rightarrow H_2 + ½ O_2$
H_2
H_2O
O_2
-xx kJ/mol
Gas-to-Liquid (GTL) chemistry
Fischer-Tropsch (FT)
methanol to gasoline (MTG)
syngas to gasoline (STG)
carbon-containing fuel
H_2O
-41 kJ/mol
$H_2O + CO \rightarrow H_2 + CO_2$
H_2
CO_2
water-gas shift reaction
reaction enthalpies calculated for gaseous products at standard conditions



Full chain of CO_2 neutral fuels
renewable energy
-xx kJ/mol
CO_2 hydrogenation
methane (Sabatier),
methanol synthesis
H_2O
reverse water-gas shift reaction
+41 kJ/mol
$CO_2 + H_2 \rightarrow CO + H_2O$
H_2O
CO
O_2
CO_2
+283 kJ/mol
$CO_2 \rightarrow CO + ½ O_2$
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Gas-to-Liquid (GTL) chemistry
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syngas to gasoline (STG)
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H_2O
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$H_2O + CO \rightarrow H_2 + CO_2$
H_2
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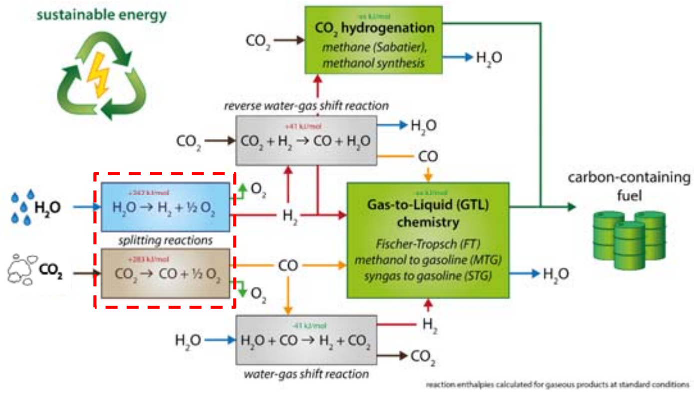
reaction enthalpies calculated for gaseous products at standard conditions

The Challenge: H_2 or CO generation



- **Use-inspired research is focused on:**
  - *H_2 generation from H_2O*
  - *CO generation from CO_2*
- **The challenge:**
  - *To find a cost-effective and energy efficient conversion process using robust and scalable materials and processes*

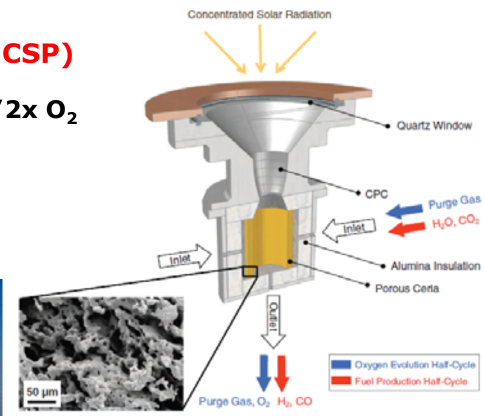
Thermochemical using CSP (direct)

Concentrated solar power (CSP)

CeO_2 + sunlight → CeO_{2-x} + 1/2x O_2

CO_2 + CeO_{2-x} → CO + CeO_2

Or based on ZnO, Fe_3O_4



Cyclic, solar to CO/H_2 efficiency: 5-7%

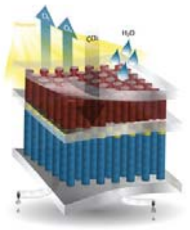
Steinfeld group (ETH Zurich), Science **330** 1798 (2010)

Photo-electrochemical Solar Fuel Conversion

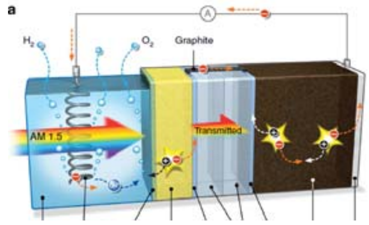
Focus on H_2 generation

Daniel Nocera Harvard/MIT

Rene Janssen TU/e-DIFFER

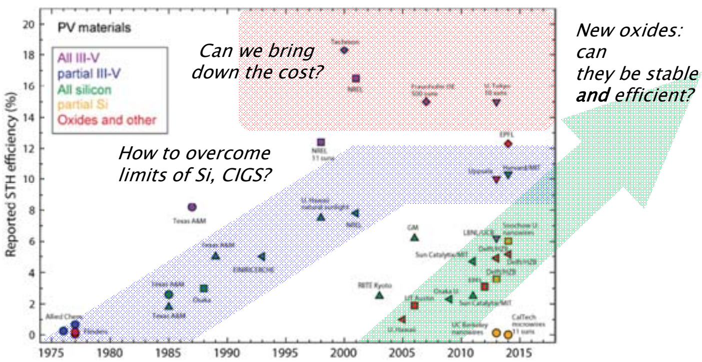


Nathan Lewis et al. JCAP



Abdi et al. Nature Commun. **4** 2195 **(2013)**

Photo-electrodes: no clear winner yet!

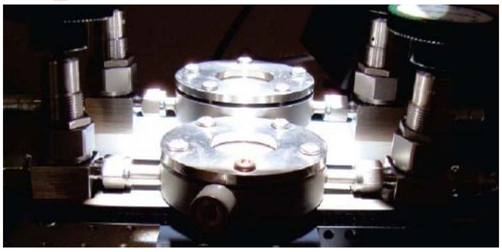


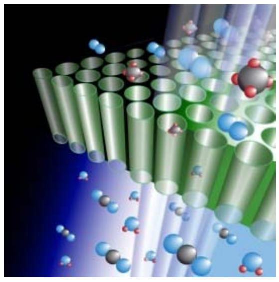
New oxides: can they be stable and efficient?

Adapted from Ager et al., *Energy & Env. Sci.* 8 (2015) 2811

Courtesy Roel van der Krol (HZB)

Photo-electrochemical conversion of CO_2 ?





TiO_x tubes with Cu catalyst

To tailor the catalyst to optimally use the solar spectrum for activating the catalyst

$CO_2 + 2H_2O \rightarrow CH_4 + 2O_2$

Solar to methane efficiency η = 0.0148%

Roy, Varghese, Paulose, Grimes, ACSNano **4**, 1260 (2010)

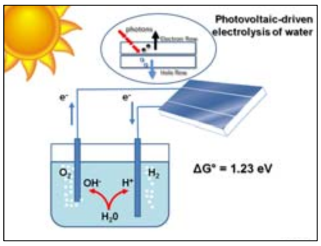
Status of H_2 generation

Photo-electrochemical/catalytic: < 0.2-6 %

Solar thermal: 5–7 %

Indirect conversion

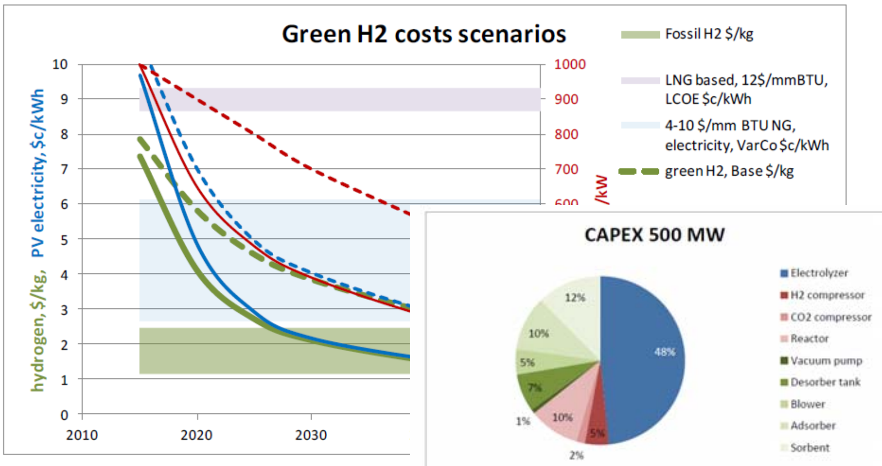
Renewable electricity + Electrolysis



Three types known

- Alkaline (liquid sodium or potassium hydroxide electrolyte)
  Slow reaction kinetics, slow response to fluctuations, large Ohmic losses
- Polymer Electrolyte Membrane (PEM) based
  Fast response, expensive catalysts, cross-over, high current densities
- Solid Oxide Membrane based
  Slow response, high temperature (700-900 ºC), material stability

Electricity to methanol: a study



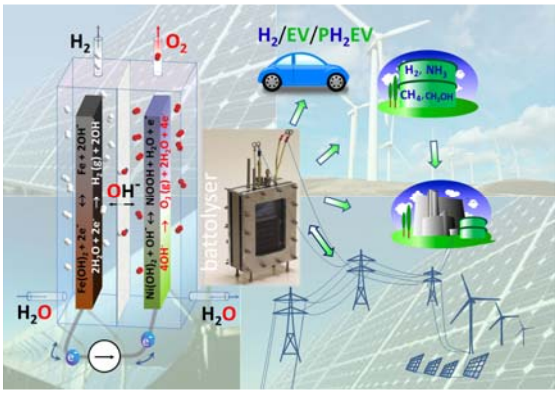
Electrolyzer: dominant cost in CAPEX

Antecy and Shell business calculation, incl. carbon capture

Battolyser

An integrated battery and electrolyser*: battolyser*

- Store electricity in the battery with high P2P efficiency
- Battery full: additional electricity is converted to H_2
- H_2 enables Haber, Sabatier & Fischer-Tropsch, Fe reduction
- 2 for 1



Fokko Mulder *et al.*, Energy & Environmental Science 2017

HOT paper

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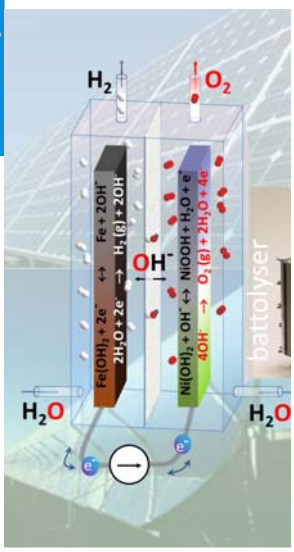
Battolyser



Basic reactions:

Negative electrode:

Battery:

$Fe(OH)_2 + 2e^- \leftrightarrow Fe + 2OH^-$

Electrolysis:

$2H_2O + 2e^- \rightarrow H_2\,(g) + 2OH^-$

Positive electrode:

Battery:

$Ni(OH)_2 + OH^- \leftrightarrow NiOOH + H_2O + e^-$

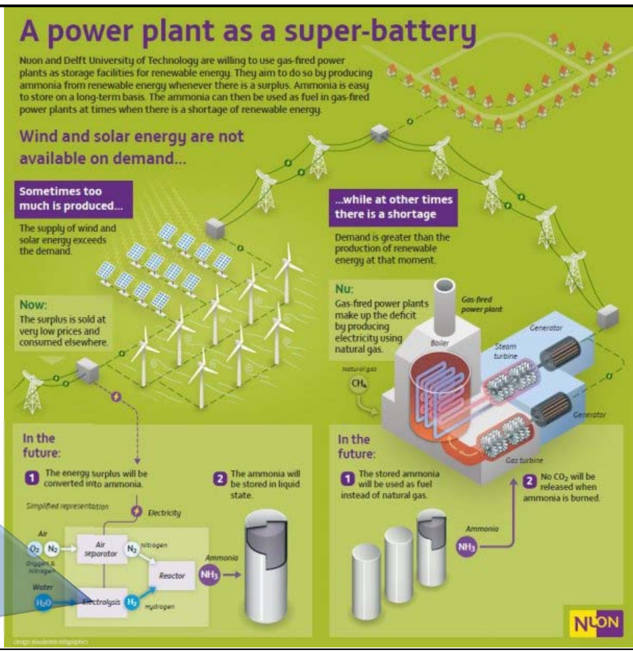
Electrolysis:

$4OH^- \rightarrow O_2\,(g) + 2H_2O + 4e^-$

TUDelft 32

and a super-battolyser

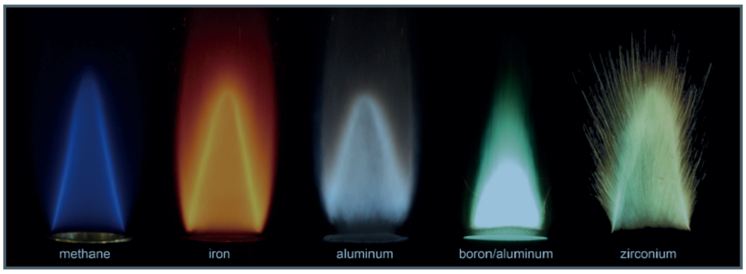
TUDelft



TUDelft

Courtesy of F. Mulder (TUD)

Metal Combustion & Reduction



Use of different types of metal powders as a fuel

JM Bergthorson, S Goroshin, MJ Soo, P Julien, J Palecka, DL Frost, and DL Jarvis. Direct combustion of recyclable metal fuels for zero-carbon heat and power. Applied Energy 160 (2015), 368-382.

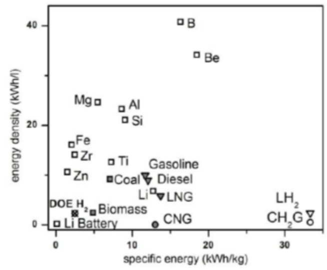
Key ideas

- Zinc (and Iron) powder combustion for electricity and transport (ships, trucks,..)
- Oxide particle capture and reduction back to metal powders using renewable energy

metalot TU/e

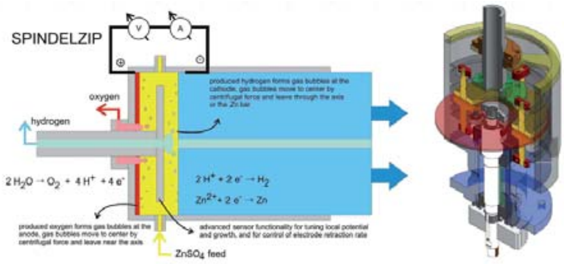
Courtesy by P. de Goey (TU/e)

Metal Fuels on Metalot Campus



- Very high energy density
- No CO_2 emissions
- Mid-term: spinning-disc technology metal production via electrolysis
- Long-term: development of metal fuels for transport, energy generation, conversion and storage

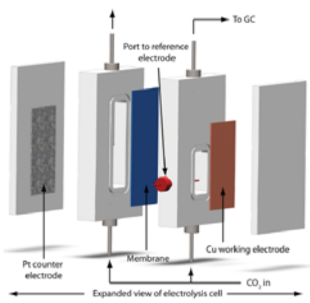
Spinning disc reactor

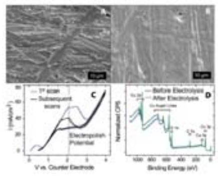


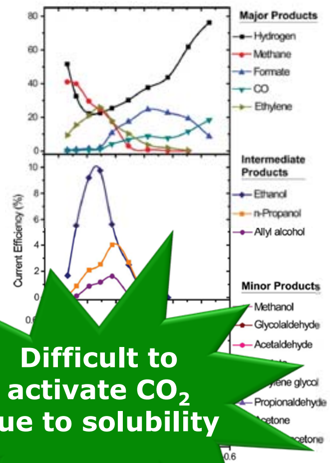
Courtesy by P. de Goey (TU/e)

metalot TU/e

CO_2 reduction ?







Electrical energy to CO > 10%

→ Electrochemic Conversion

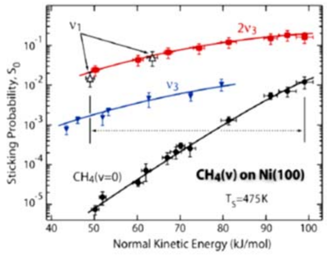
Difficult to activate CO_2 due to solubility

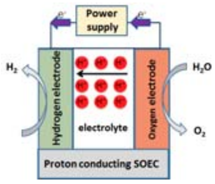
K.P. Kuhl et al., Energy Environ. Sci. **5** 7050 (2012)

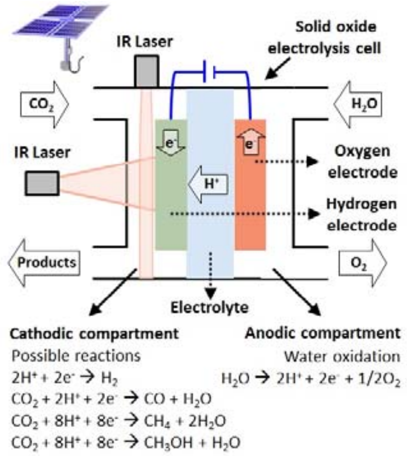
NWO

New approach: internally excited molecules

Co-electrolysis of CO_2/H_2O



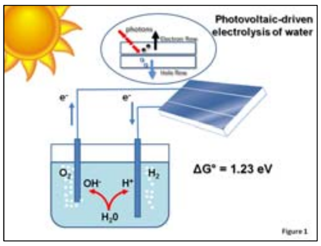




F. Fleming Crim, 'Chemical dynamics of vibrationally excited molecules: Controlling reactions in gases and on surfaces" PNAS, 2008, 105, 12654-12661

Challenges (indirect conversion)

Renewable electricity
+
Electrolysis



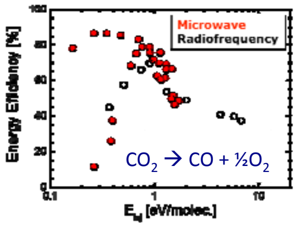
Indirect Solar-to-chemical energy conversion

- Focused on cost efficient materials and materials synthesis
  e.g. polymer membranes for polymer membrane electrolysis, novel abundantly available catalysts
- Novel innovative operational concepts
  e.g. system integration and intermittency, heat integration and co-electrolysis for high pressure solid oxide electrolysis

Challenges (indirect conversion)

Renewable electricity + Plasmolysis

CO_2 recycling



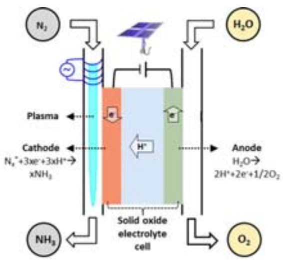
A. Fridman *Plasma Chemistry*

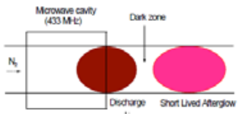
Indirect Solar-to-chemical energy conversion

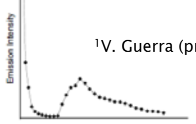
- Focused on cost efficient materials and materials synthesis
  e.g. polymer membranes for polymer membrane electrolysis
- Novel innovative operational concepts
  e.g. system integration and intermittency, heat integration and co-electrolysis for high pressure solid oxide electrolysis
- To overcome these challenges for electrolysis:
  alternative indirect approach based the generation of a non-equilibrium plasma using renewable electric energy

Plasmo-electrochemical membrane reactor

Ammonia synthesis







For a non-equilibrium nitrogen discharge as much as **70-80%** of the power input ends up in internal excitation[1]

[1]V. Guerra (private communication)

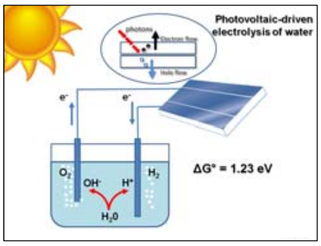
Combination of vibrational (plasma) excitation and electrocatalysis for N_2/H_2O

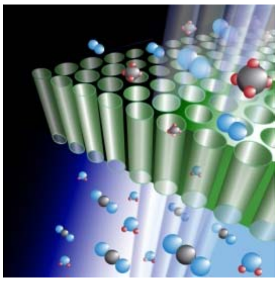
Note that both plasma and membrane reactor are driven by renewable electricity!!

M. Tsampas (DIFFER)

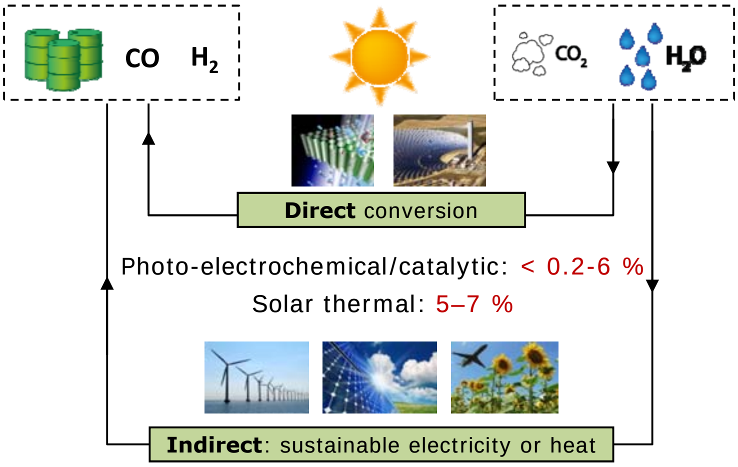
Contents

- **The Energy Transition**
  - Greening the (chemical) industry
  - Electricity to fuels, feedstock
- **P2G;P2L;P2X; (P2Heat)**
- **Summary**





Status of H_2 generation



Electrochemistry for H_2 production: (25%)×(70-80%) = 18-20%

Summary

- **The Energy Transition**
  - Electricity to chemistry (fuels, feedstock) is going to be an key enabling technology: P2G, P2L, P2X,… for a future CO_2 neutral society
- **Various approaches exist, in different stages of development:** electrolysis most mature
- **At the moment no cost-efficient approach available if compared with fossil feedstock based approaches**
- **Long term research & development needed: incremental and disruptive approaches**
  - Electrolysers: materials, integration and upscaling (“science of making”)
  - Electrochemistry: H_2O/CO_2 co-electrolysis, ammonia production, etc.
  - Artificial leafs, (photo-)thermochemical conversion, non-thermal approaches (plasmolyse/plasma, plasmon resonance induced chemistry, etc.)