The Transformation of the Chemical and Related Industries towards CO_2-Neutrality

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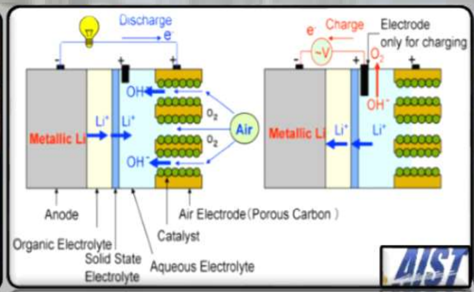
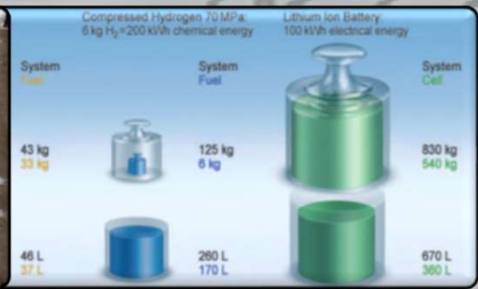
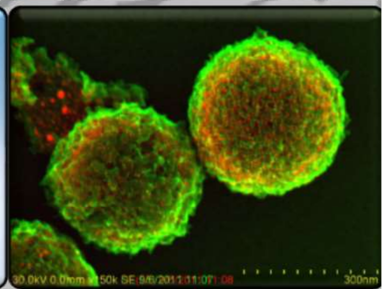
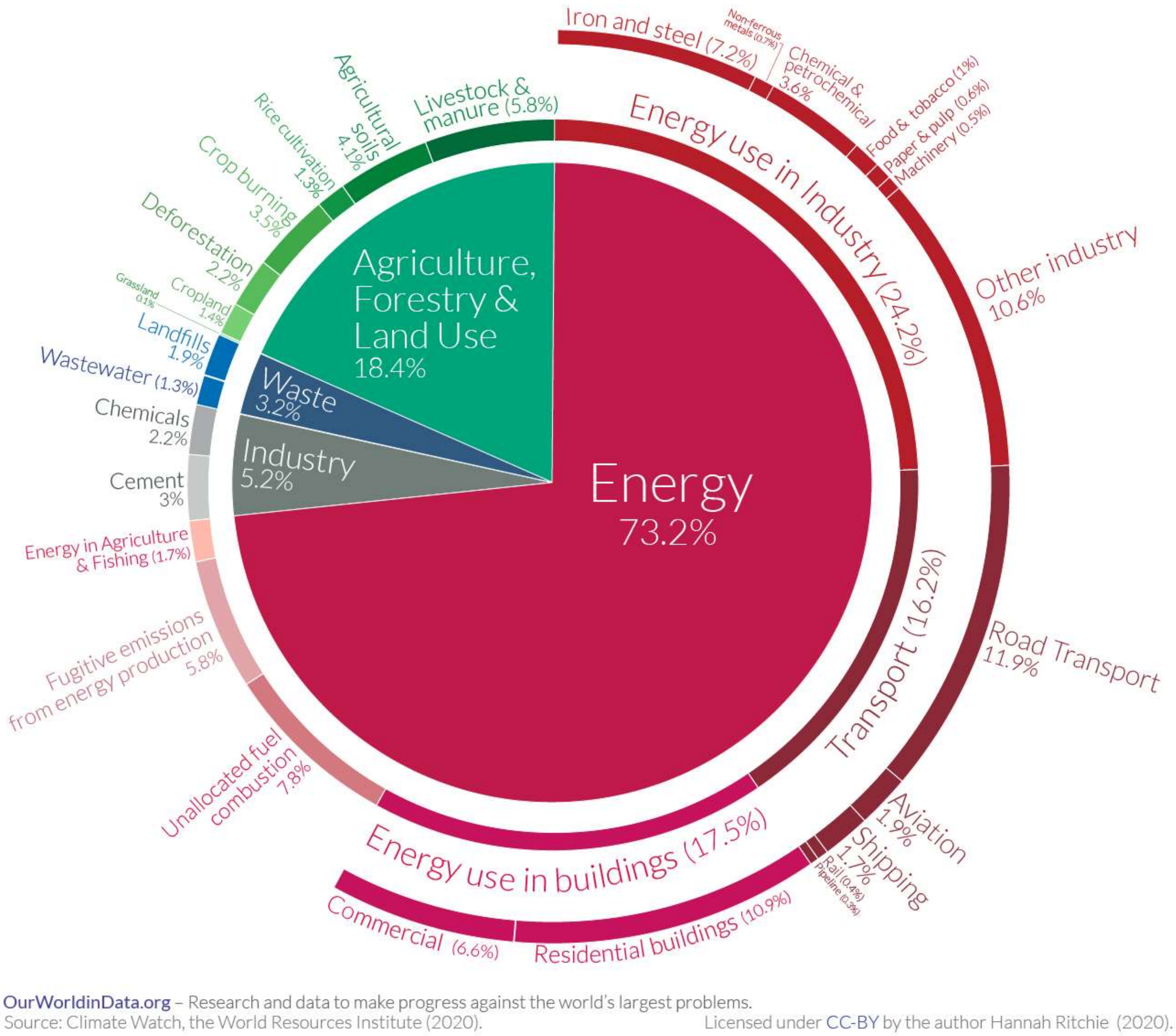


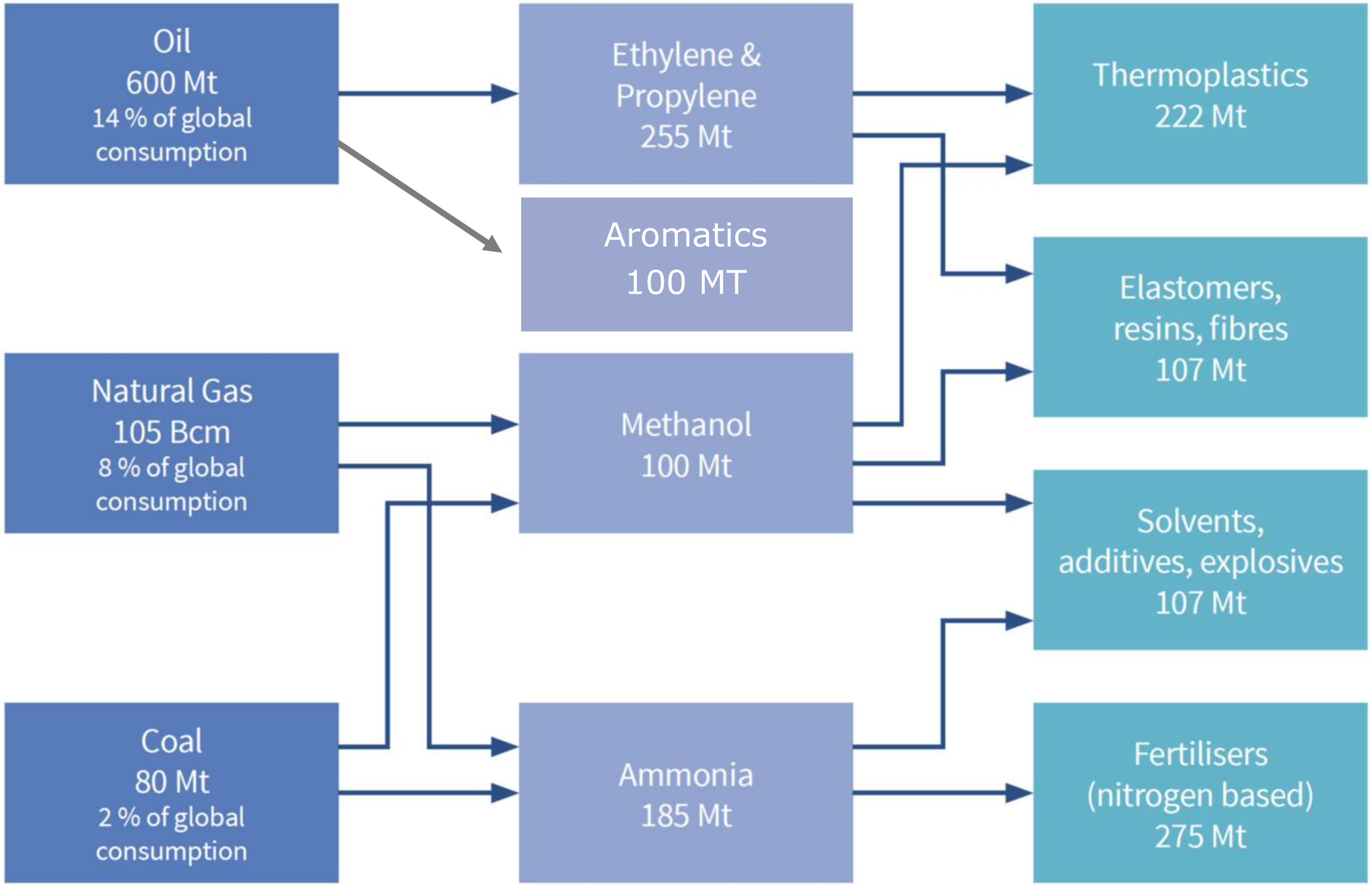




Breakdown of global greenhouse gas emissions



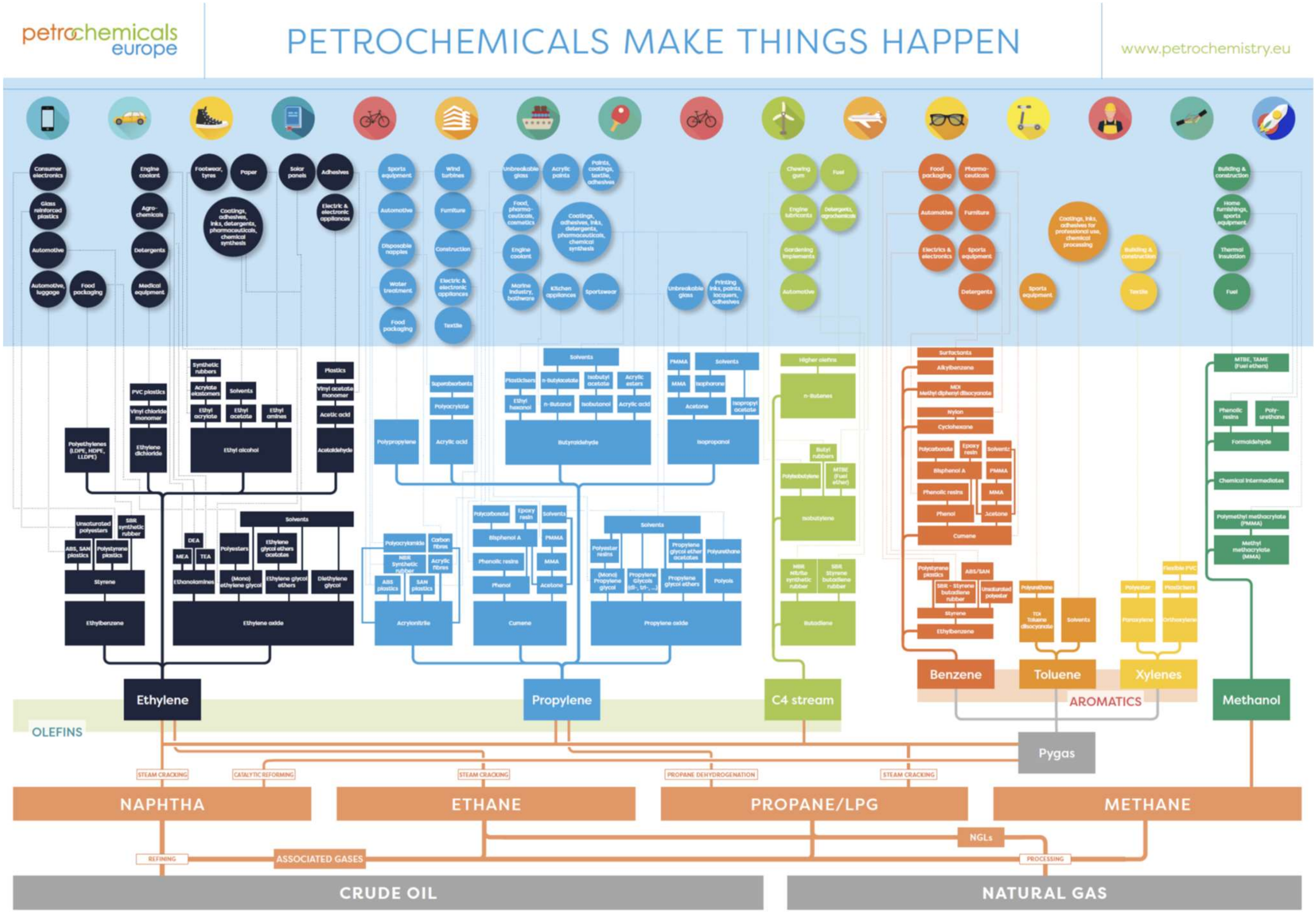
What is the basis?



Source: IEA, 2018

Roughly half of the input used as raw materials

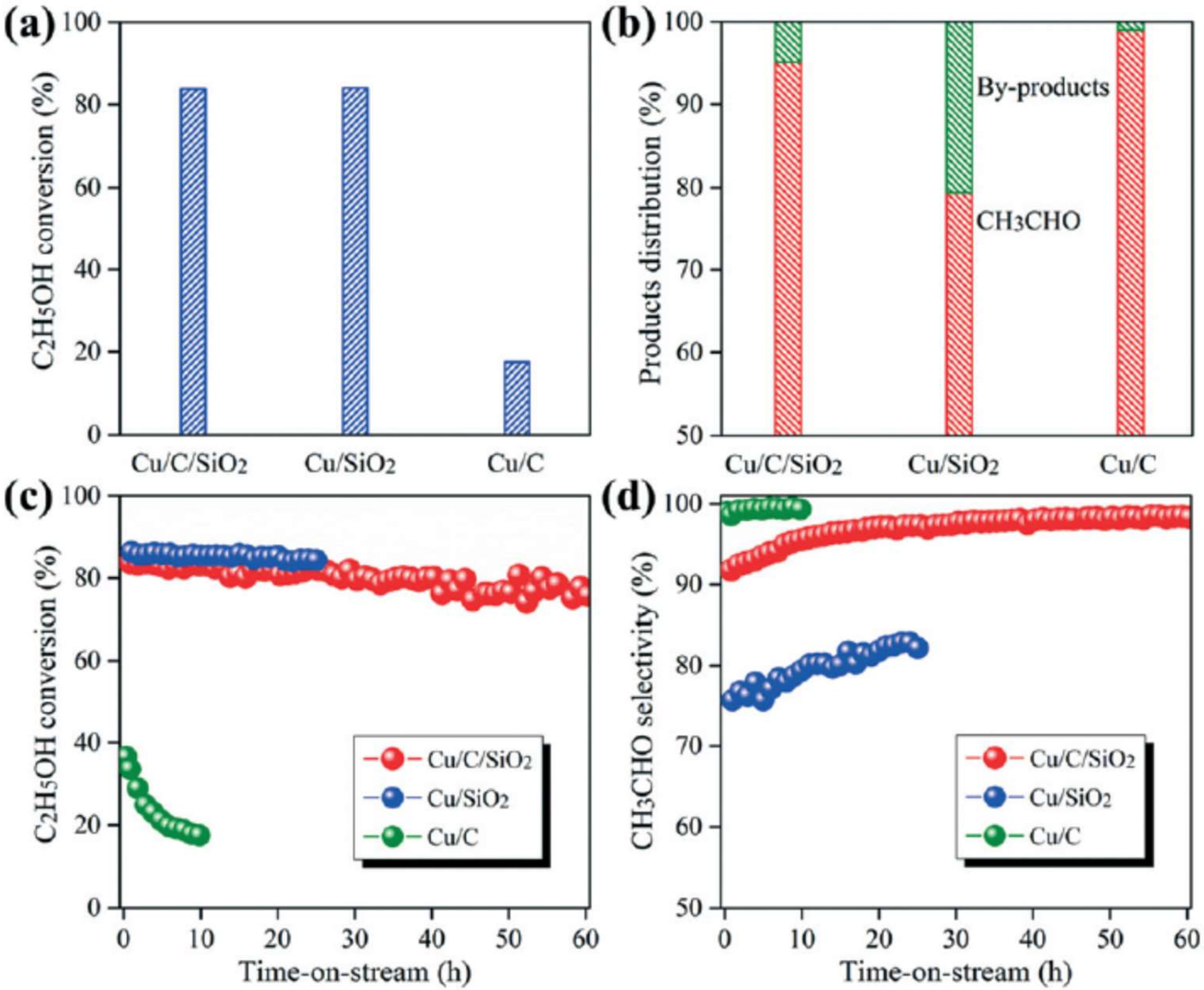
Petrochemicals flow chart

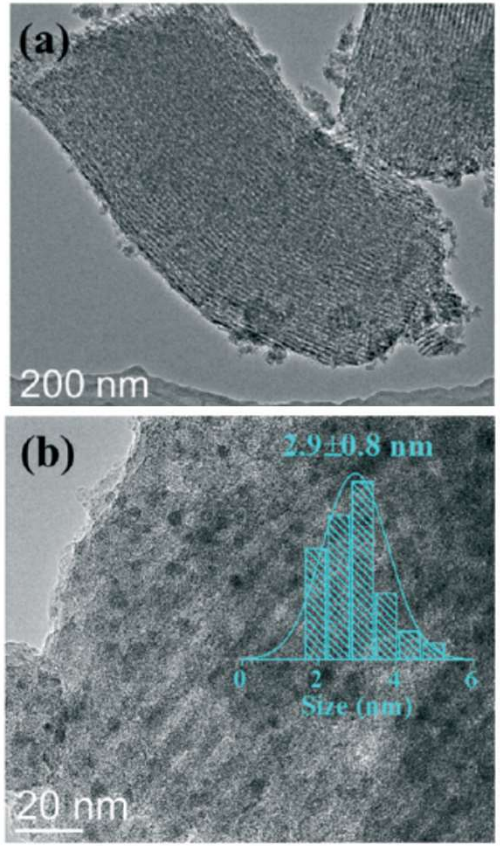


https://www.petrochemistry.eu/about-petrochemistry/flowchart/

Single processes to renewables basis: acetaldehyde from ethanol

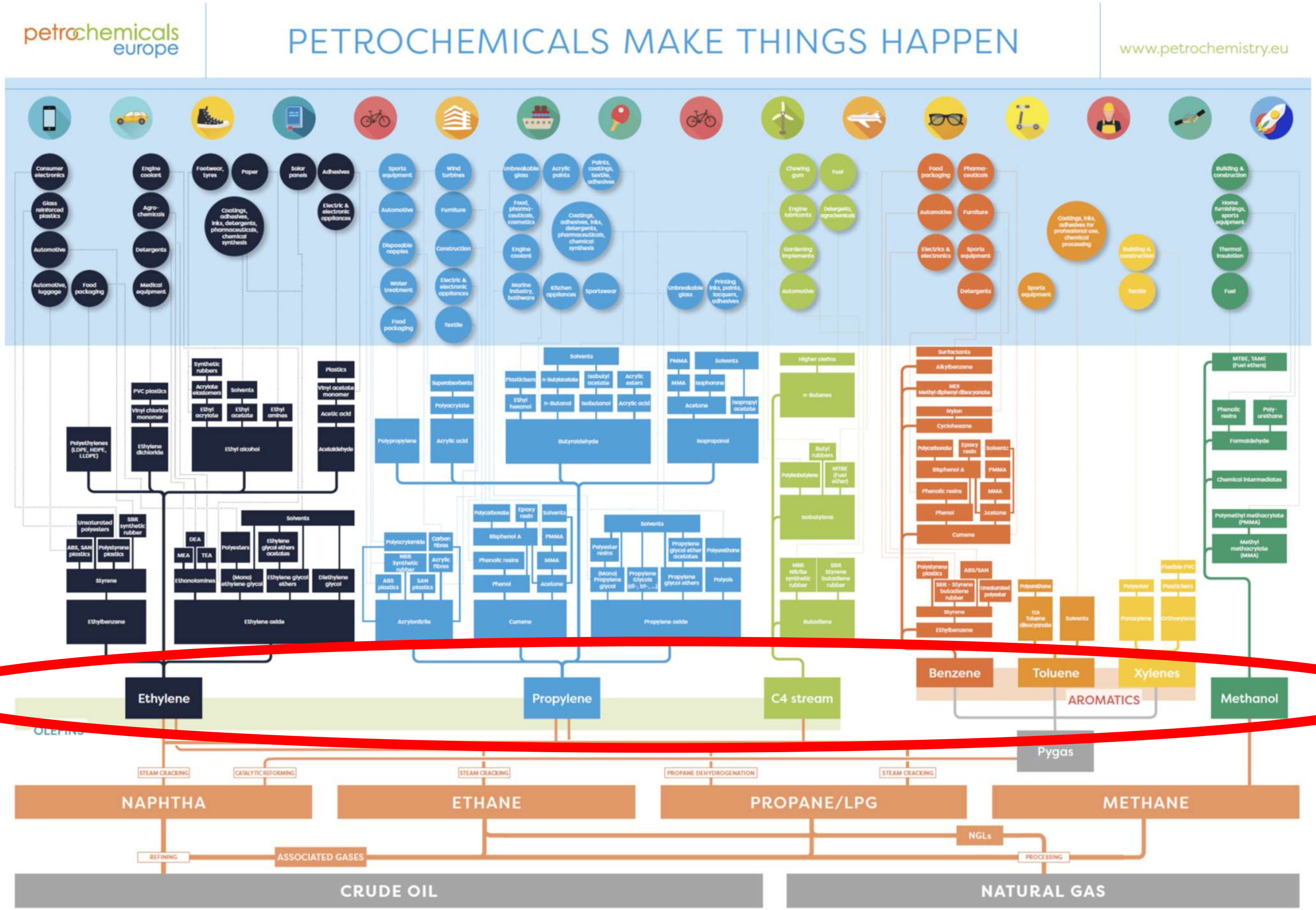
$$C_2H_5OH \longrightarrow C_2H_4O + H_2$$





Q.N.. Wang,…A.H. Lu, Catal.Sci.Technol. 8, 472 (2018)

Petrochemicals flow chart



https://www.petrochemistry.eu/about-petrochemistry/flowchart/

Essential fields of action

- **Novel feedstock (biomass, CO_2, waste)**

- **Electrification**

- **Novel processing**

CO_2 first of course from concentrated sources, i.e. combustion, biogas!

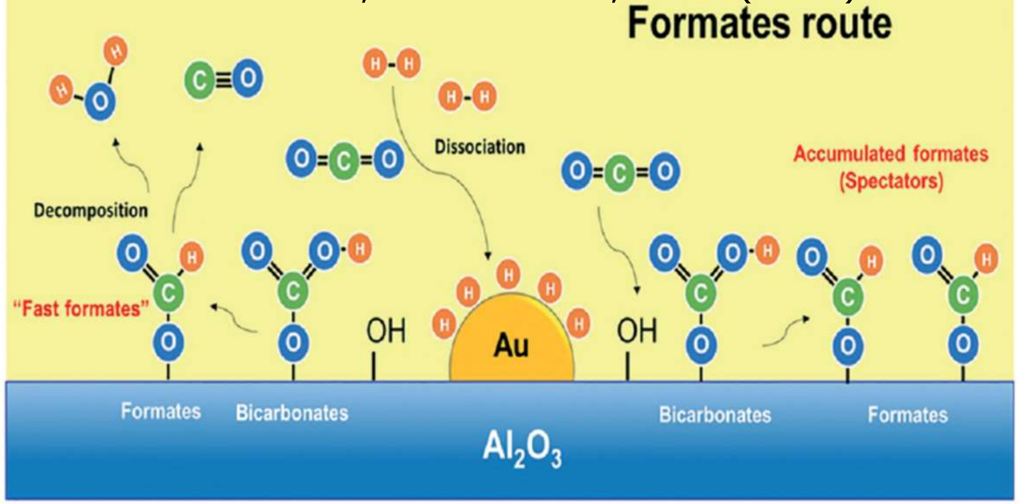
Realized in Iceland by Climeworks

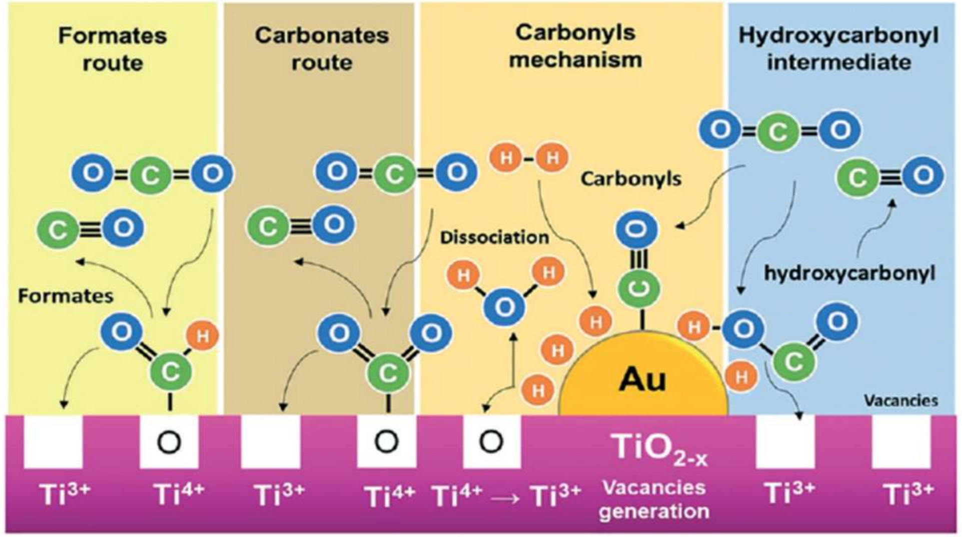
D.W. Keith et al., Joule 2,1573 (2018)

CO_2-to-hydrocarbons

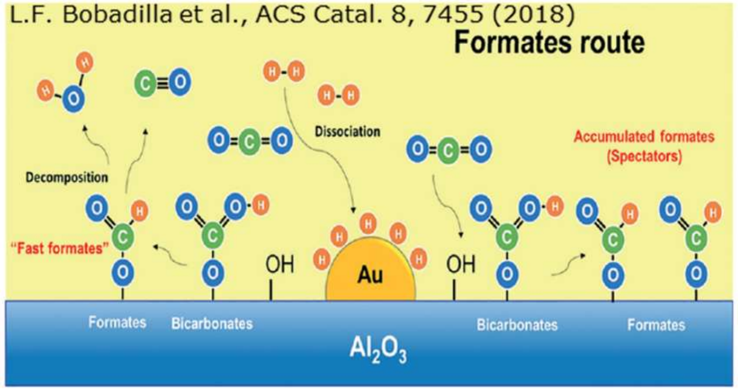
- **Aviation fuel will not be replaced by electrical energy or hydrogen (although Airbus plans hydrogen powered jet by 2035…)**
- **„Past fossil" jet fuel: Jet-fuel accessible by syngas chemistry**
- **Regulatory ok, since syngas based jet fuel approved**
- **Problem for large scale implementation of CO_2-neutral route: reverse water-gas shift: see M. Gonzalez-Castano et al. Reaction Chemistry and Engineering 6, 954 (2021)**

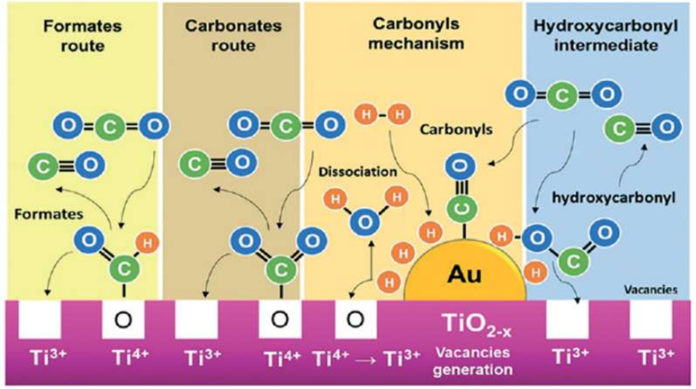
L.F. Bobadilla et al., ACS Catal. 8, 7455 (2018)





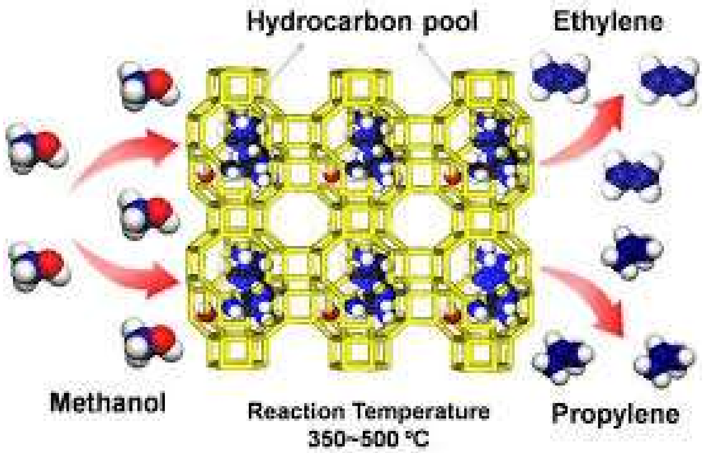
CO_2-to-methanol-to-olefins to replace steam cracker





- **After reverse water-gas-shift: methanol synthesis**
  Alternative: direct CO_2 hydrogenation to methanol

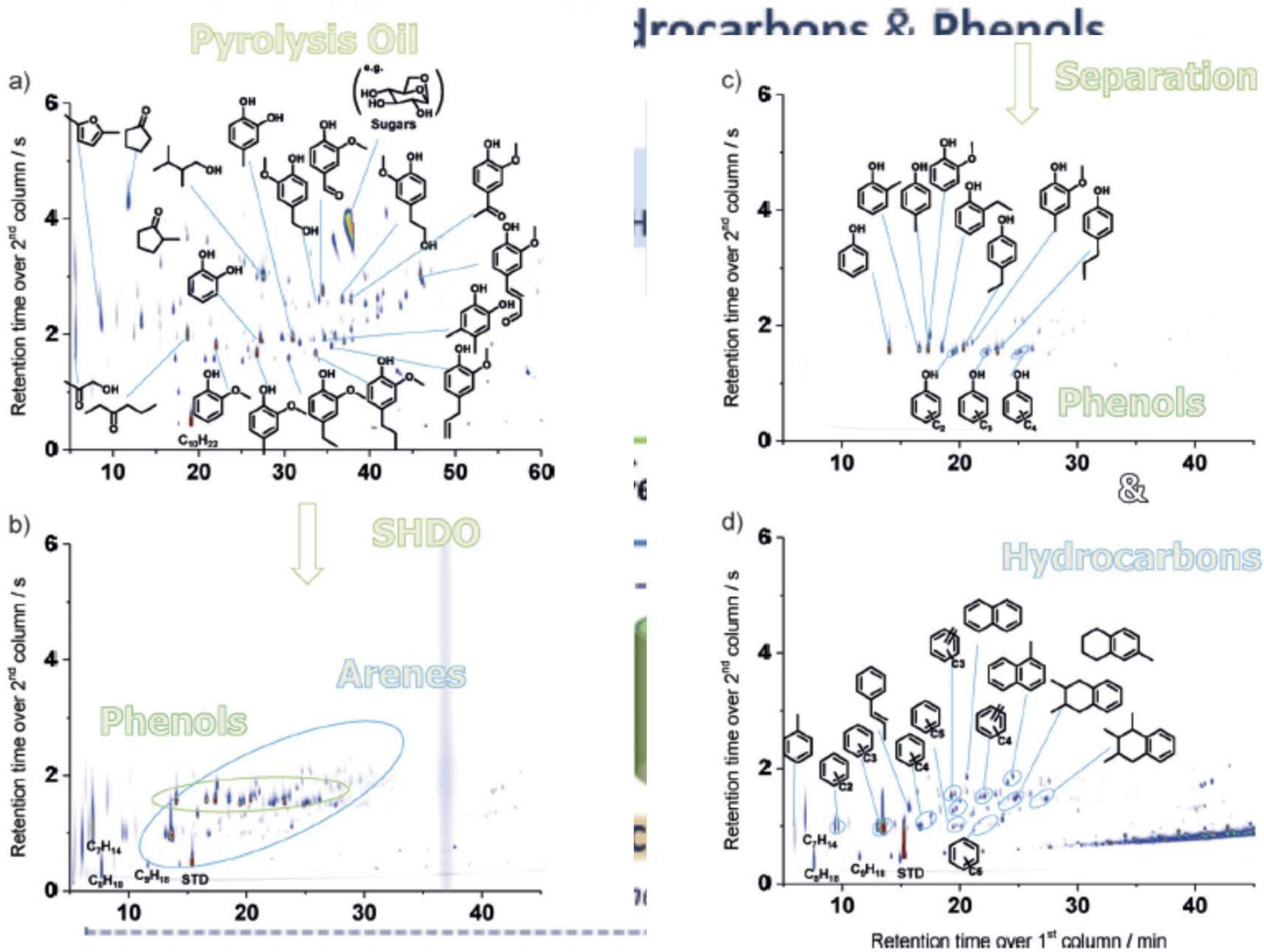
- **Then methanol-to-olefins (MTO)**



Ethene to propene adjustable
Between appr. 0.7 and almost
100% propene (Lurgi MTP process)

Possible novel technology: syngas to olefins or oxygenates

The aromatics platform from pyrolysis oil

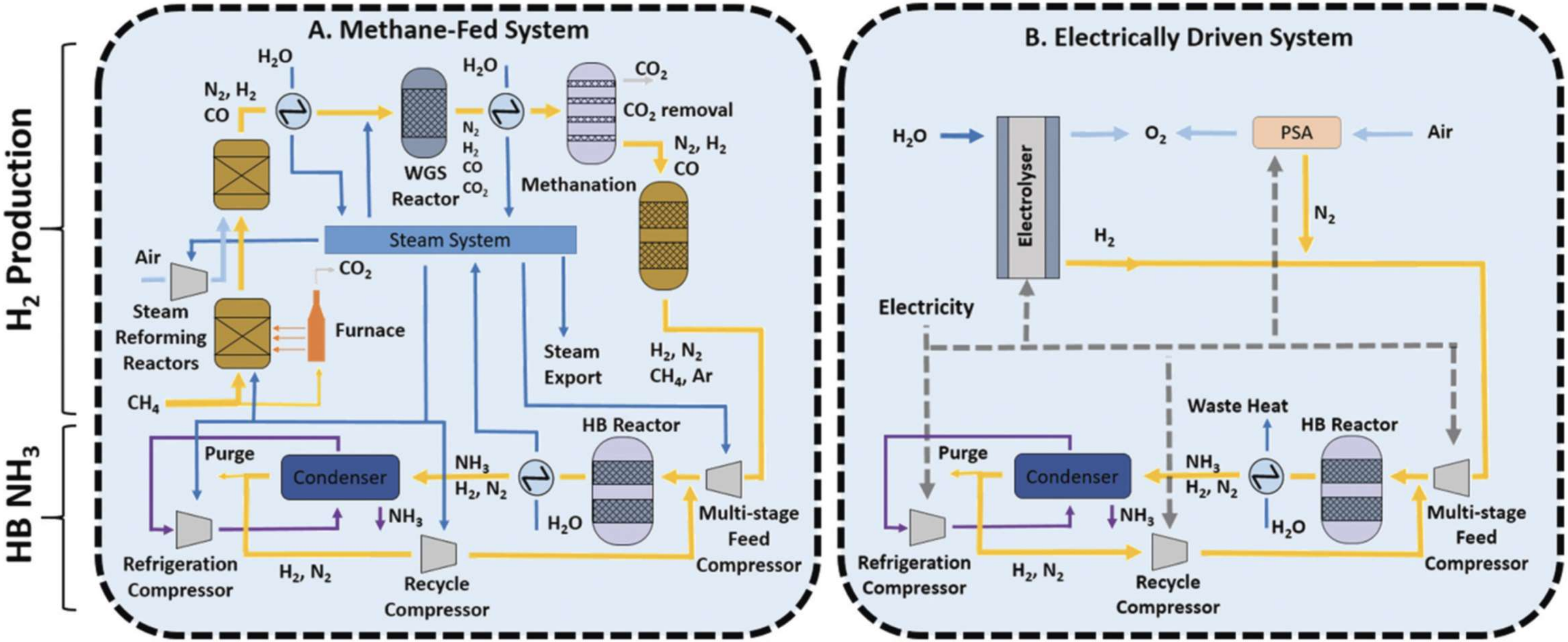


Z. Cao et al., Angew.Chem.Int.Ed. 56, 2334 (2017)

Ammonia synthesis

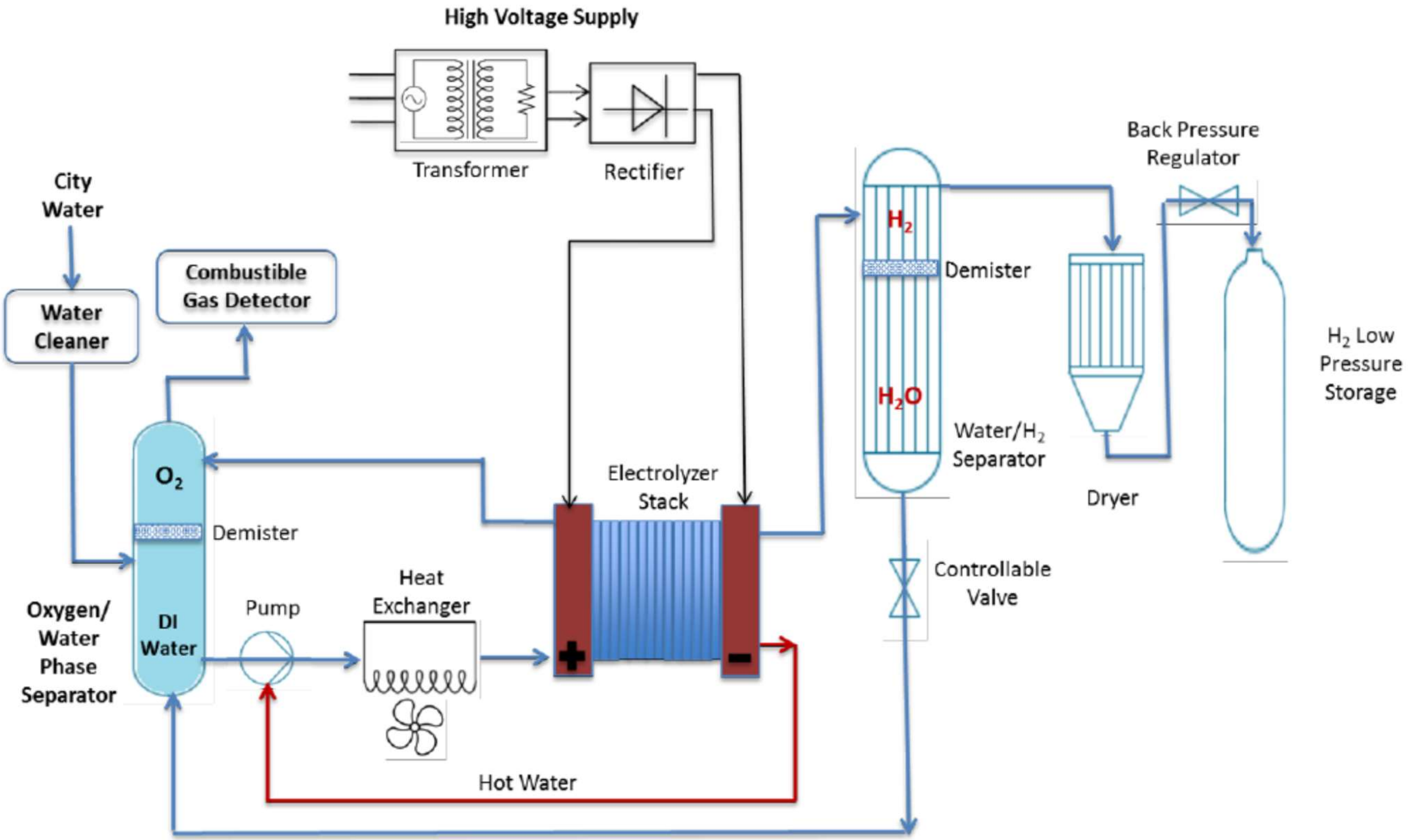
Today

The future?



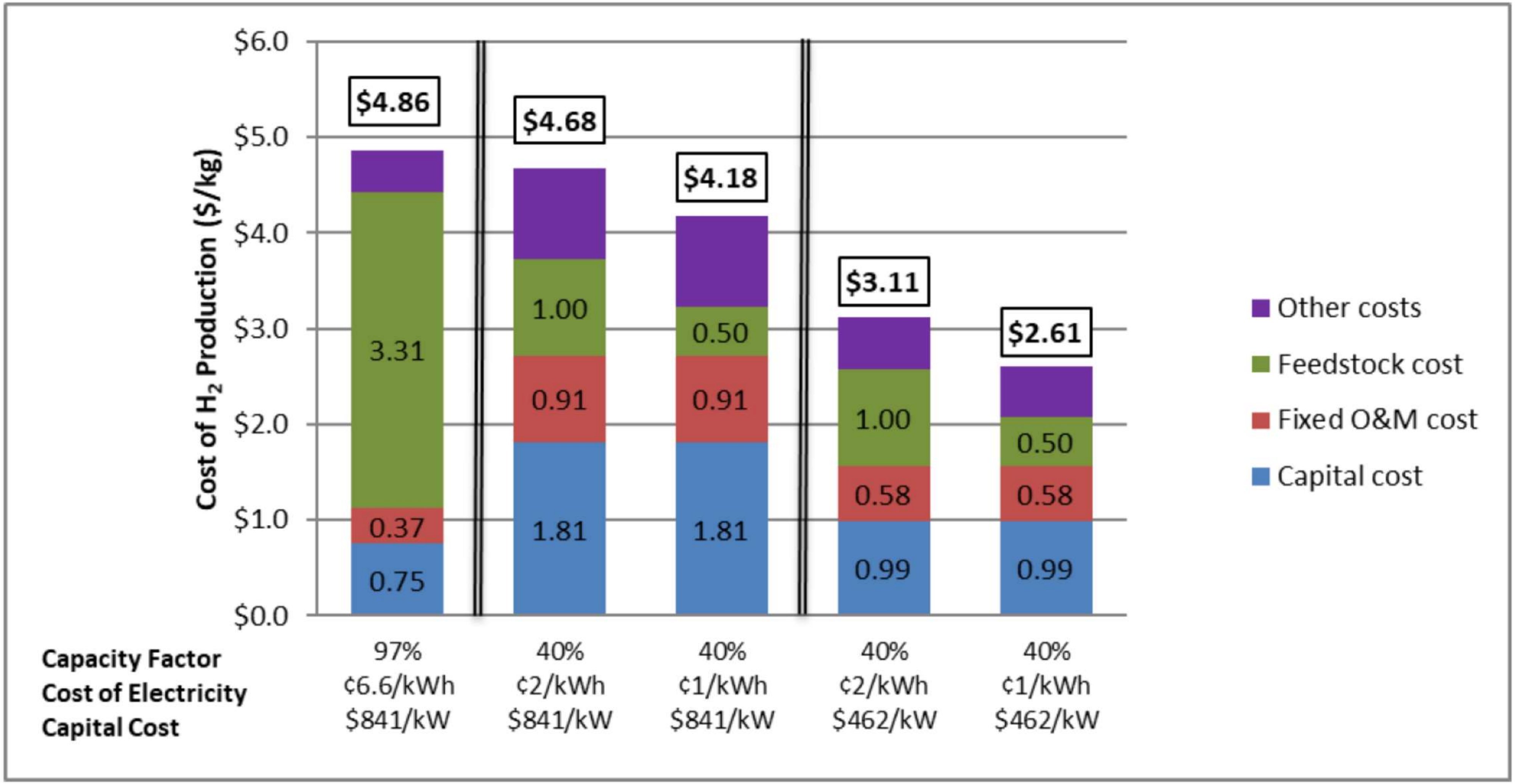
C. Smith, A.K. Hill, L. Torrente-Murciano, Energy Environ. Sci. 2020, 13, 331

Electrolyzer system



Mayyas, Ahmad, Mark Ruth, Bryan Pivovar, Guido Bender, and Keith Wipke. 2018. Manufacturing Cost Analysis for Proton Exchange Membrane Water Electrolyzers. Golden, CO: National Renewable Energy Laboratory. NREL/TP-6A20-72740, August 2019. https://www.nrel.gov/docs/fy10osti/72740.pdf.

Cost factors in electrolysis



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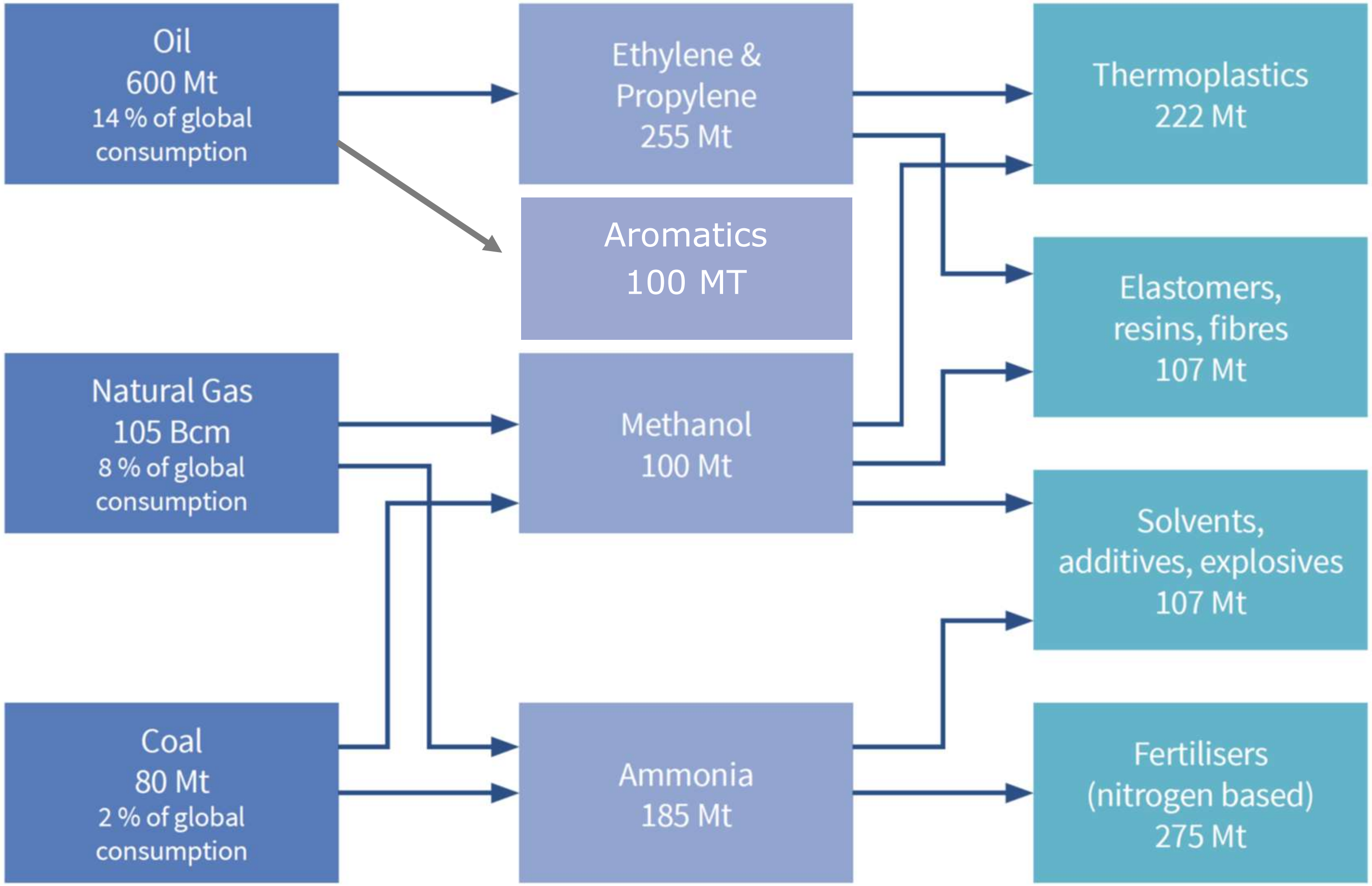
Adding up hydrogen demand (very roughly...)



Source: IEA, 2018

Roughly half of the input used as raw materials

Adding up hydrogen demand (very roughly...)

Methanol, methanol to olefins, ammonia (HDO of biooil not included)

$CO_2 + 3\ H_2 = CH_3OH + H_20$

ca. 600 Mt MeOH ca 100 MT H_2

ca. 30 Mt H_2 for NH_3

130 Mt H_2/a

50 MWh electricity /t H_2

130 000 000 x 50 MWh = 6 500 TWh/a additional electricity

German electricity production ca. 550 TWh/a

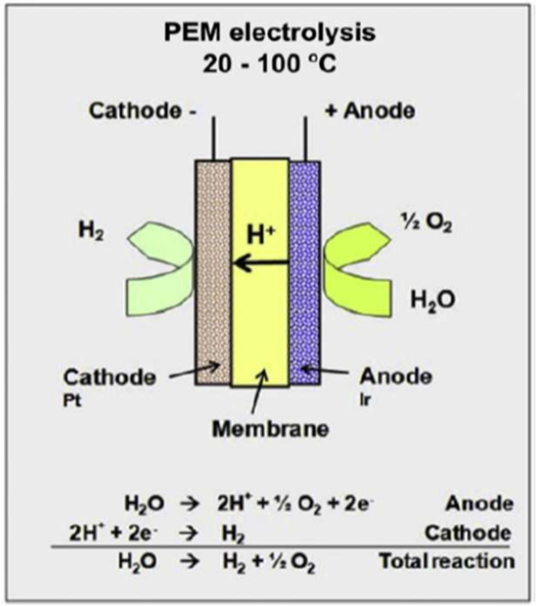
Global electricity production ca. 24 000 TWh

Converting chemical production corresponds to roughly ¼ additional global electricity demand

Electrification of chemical production

- **Process heat**

- **Synthesis with electricity**
  - **H_2 from electrolysis instead of methane reforming**
  - **FDCA from biomass**
  - **…**



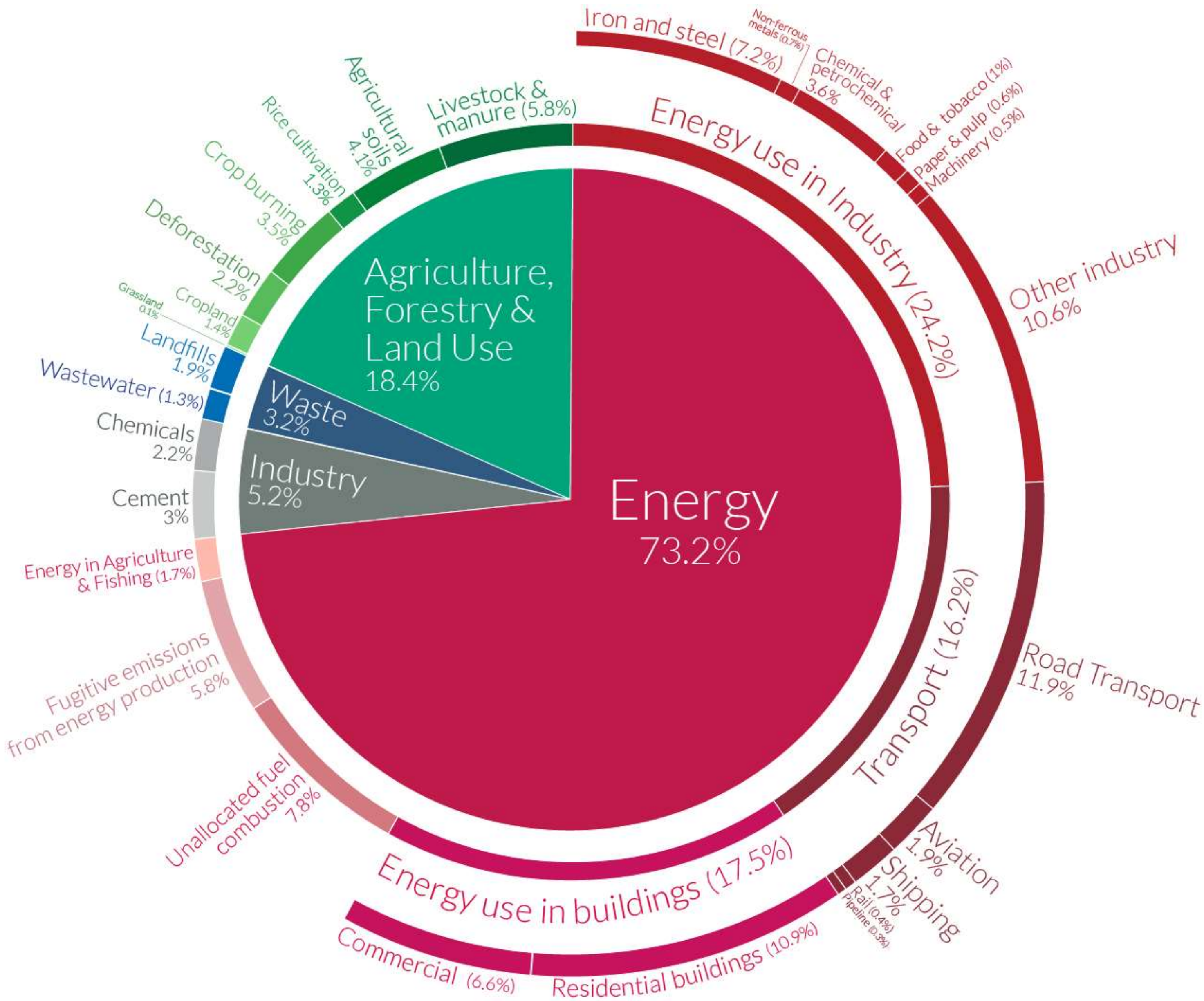
Already today: electricity consumers in chemical industry

- **Example: chlorine production in Germany (appr. 4 Mio. t) corresponds to one big power plant**

http://www.bayertechnology.com/uploads/pics/chlorine_electrolysis_service2.jpg

- **Non-steady operation ofter not economical due to unfavorable split between capex and opex**
- **Great example for non-oxygen anode reaction**

Breakdown of global greenhouse gas emissions



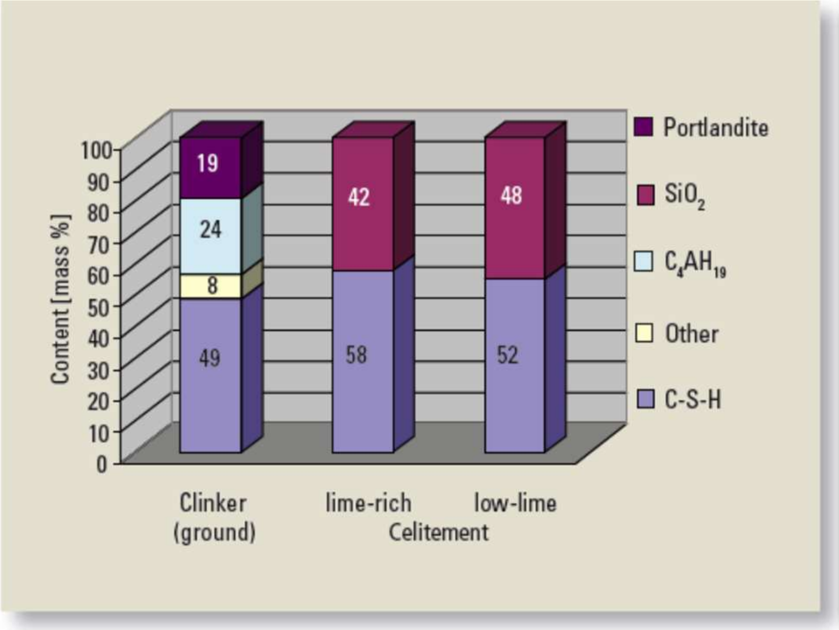
OurWorldinData.org – Research and data to make progress against the world's largest problems.
Source: Climate Watch, the World Resources Institute (2020).

Inorganics: novel cements

Inorganics generally easier to recycle: recover elements and use energy

But problematic cases, for instance cement:

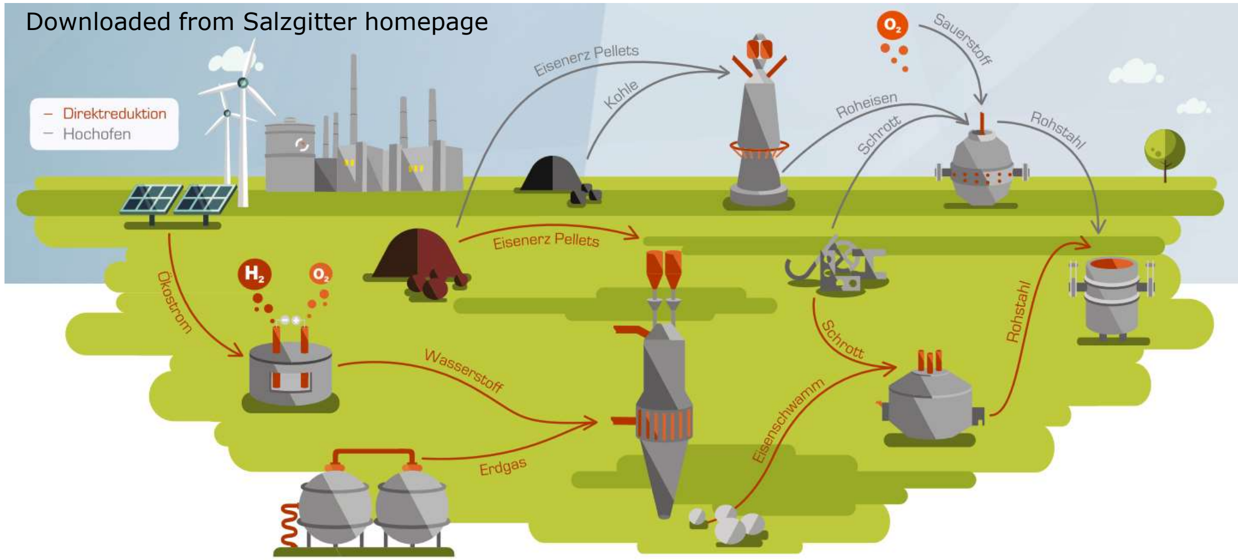
- Formation of C-S-H-phases decisive
- These have CaO/SiO_2 maximum 1.25
- More CaO in cement than would be needed
- Novel cements with low CaO content under development



P. Stennemann et al., Cement International 8, 52 (2010)

Hydrogen for the steel industry

- **At 60 kg H_2 per ton of steel: 2.4 Mt/yr in Germany**
- **At 50 MWh/t H_2 corresponds to about 60 TWh, i.e. 20% of Germany's electricity consumption**
- **Savings potential of about 70 Mt CO_2/yr**
- **Hydrogen could already reduce CO_2 footprint via steam reforming**



- **But: direct natural gas reduction is viable alternative**

Polymer recycling

nature catalysis

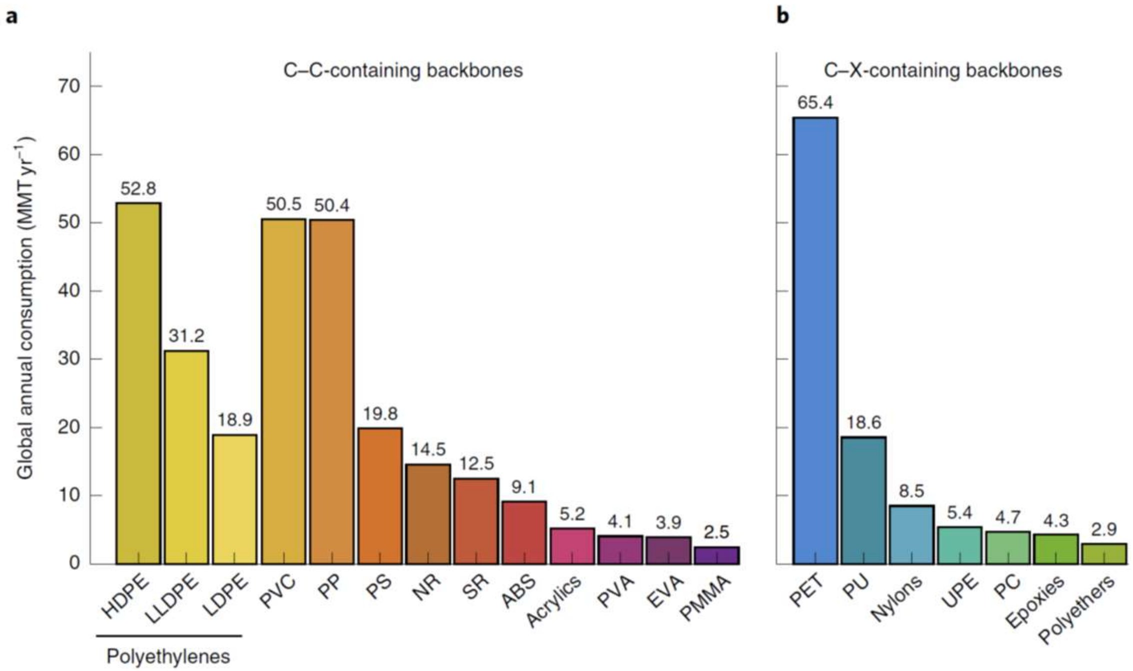
REVIEW ARTICLE

https://doi.org/10.1038/s41929-021-00648-4

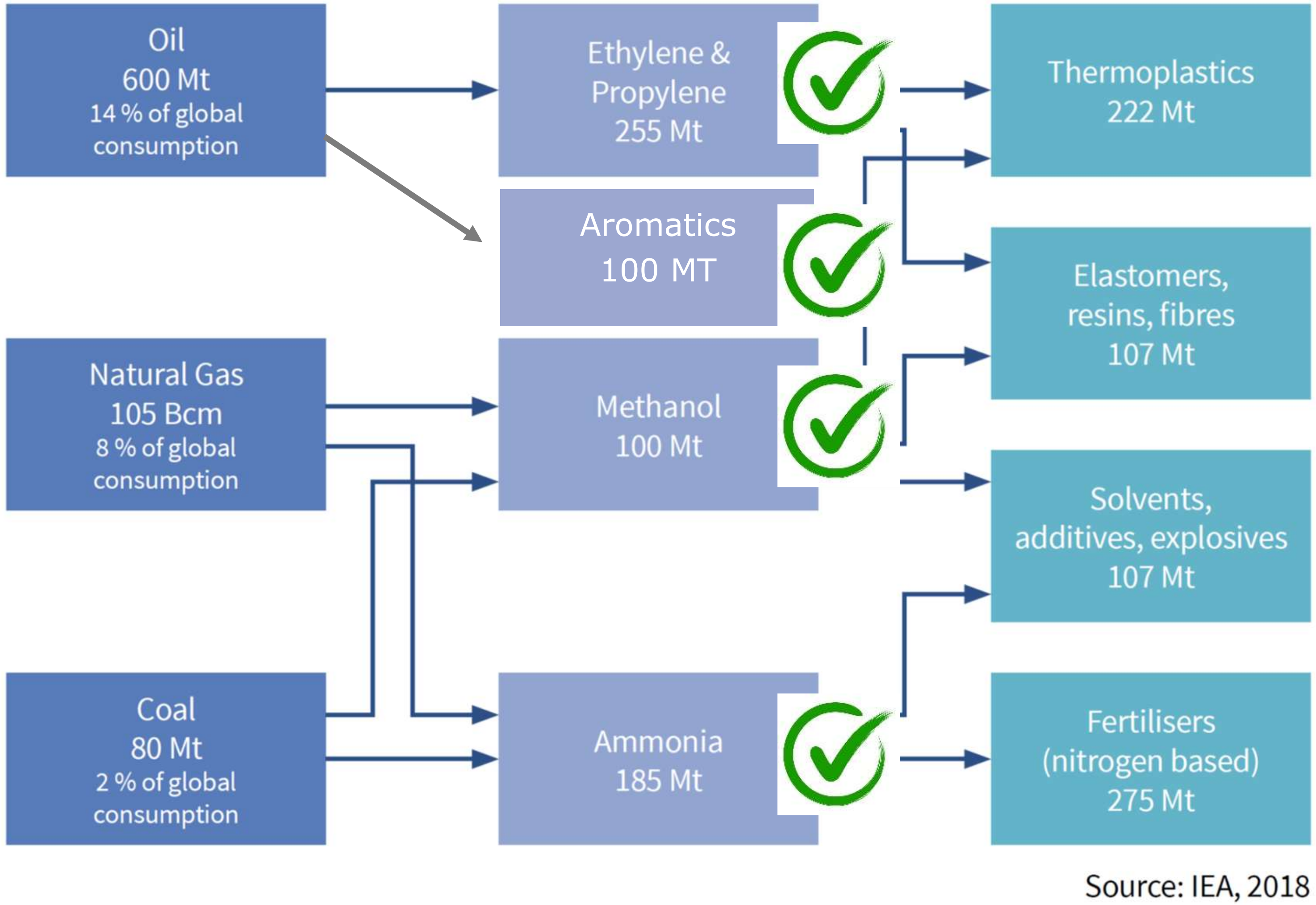
Check for updates

Chemical and biological catalysis for plastics recycling and upcycling

Lucas D. Ellis[1,5], Nicholas A. Rorrer[1,5], Kevin P. Sullivan[1,5], Maike Otto[2], John E. McGeehan[3], Yuriy Román-Leshkov[4], Nick Wierckx[2] and Gregg T. Beckham[1]



Can we convert chemical production?



- Electrification of heaters, blowers, etc.
- Direct electrification of processes/electrosynthesis

Most important element: renewable hydrogen at low cost