The Fuel Science Center 2025+

Adaptive Conversion Systems for Renewable Energy and Carbon Sources

PI-Workshop | Follow-Up Proposal 2025+

07.06.2023

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Structure of the Research Program: Examples for new ‘TRT’s

Competence Areas

CA1: Molecular Transformations and Interactions	CA2: Interfacial Phenomena and Devices	CA3: Fuel Design and Sustainable Cross-sectorial Value Chains

Translational Research Teams (TRTs)

- Ammonia Combustion (1)
- Carbon-based (drop-in) Fuels (2)
- Liquid Energy Carrier for Fuel Cells (3)
- Anti-Fragile Cross-Sectoral Systems Through Diversification and Parallelization (4)
- Integrated CO_2 Capture & Conversion (5)
- Sustainable Building Blocks, Monomers & Solvents (6)
- .....

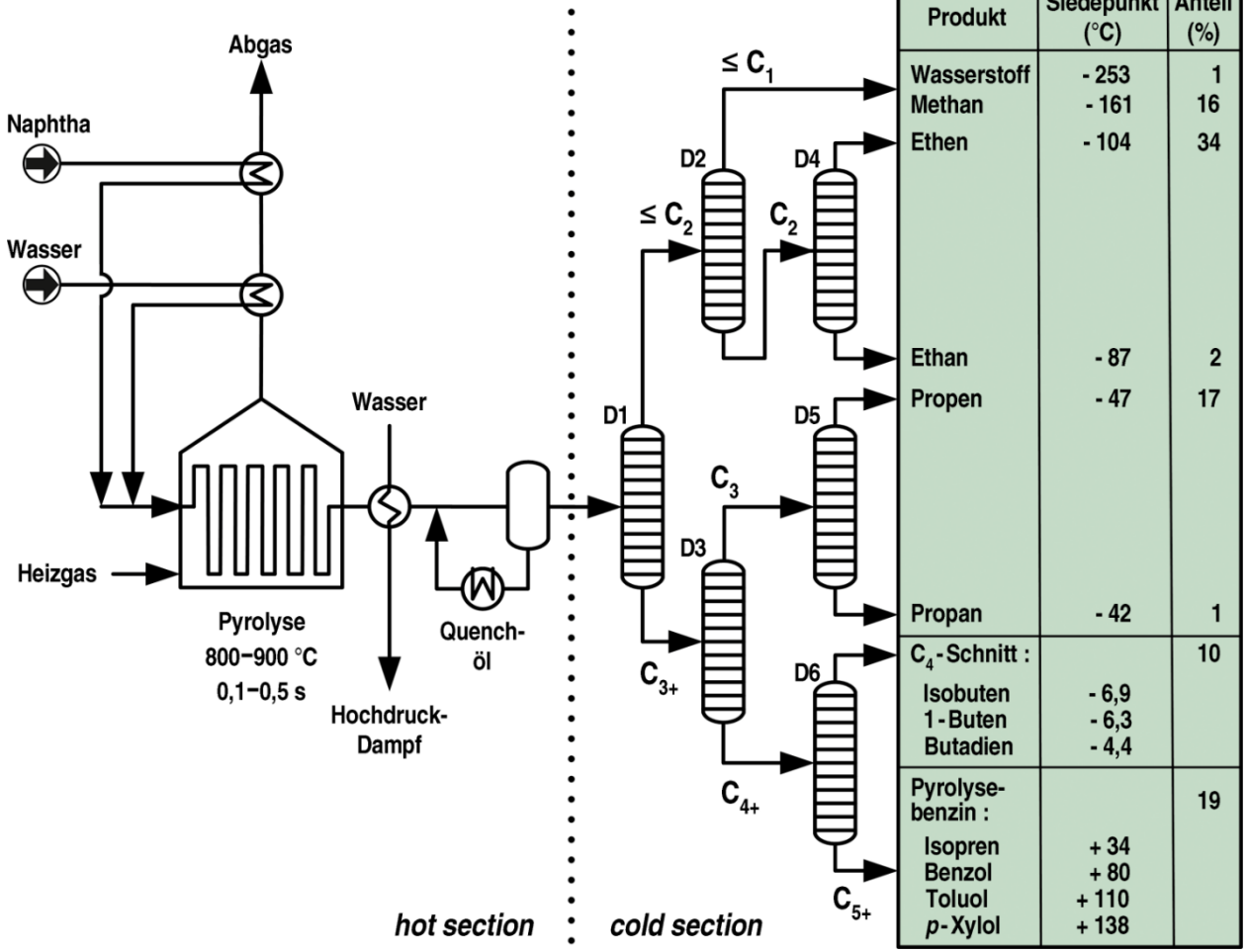
Systems Design Forum

Molecule	**Device**	**System**

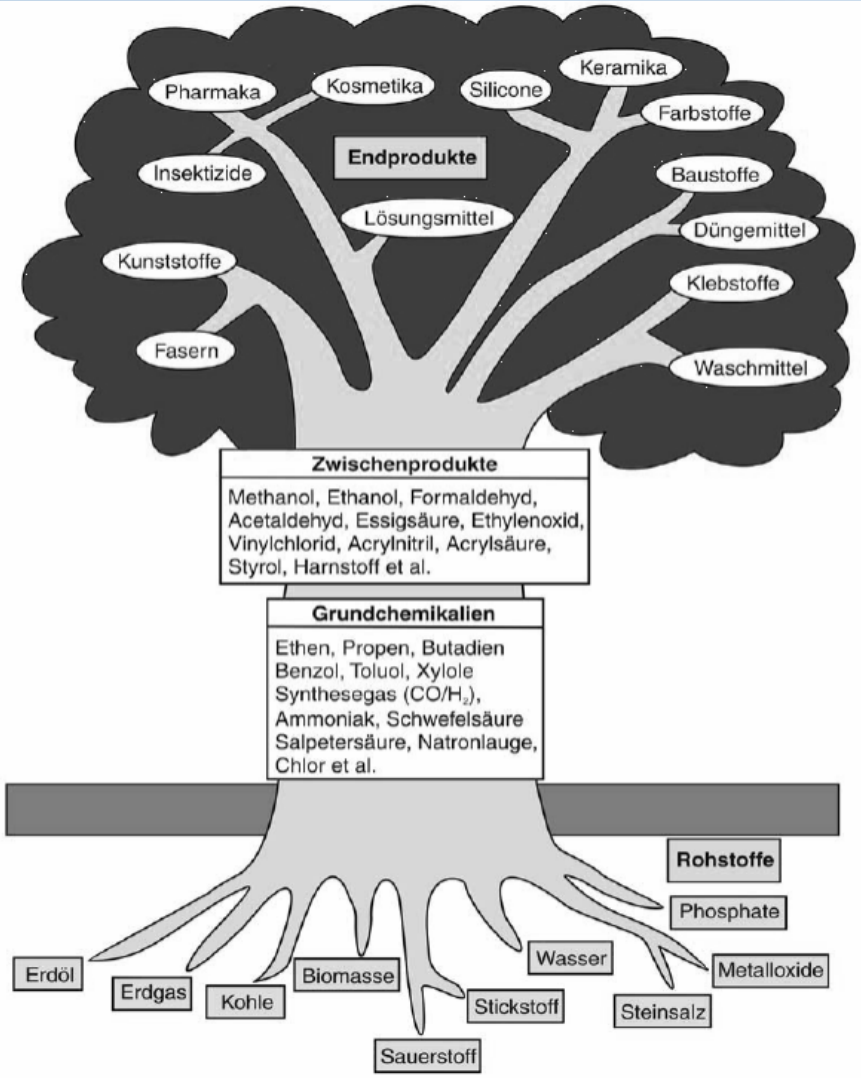
Sustainable Building Blocks, Monomers & Solvents

Basis of chemical Industry today

Steamcracker

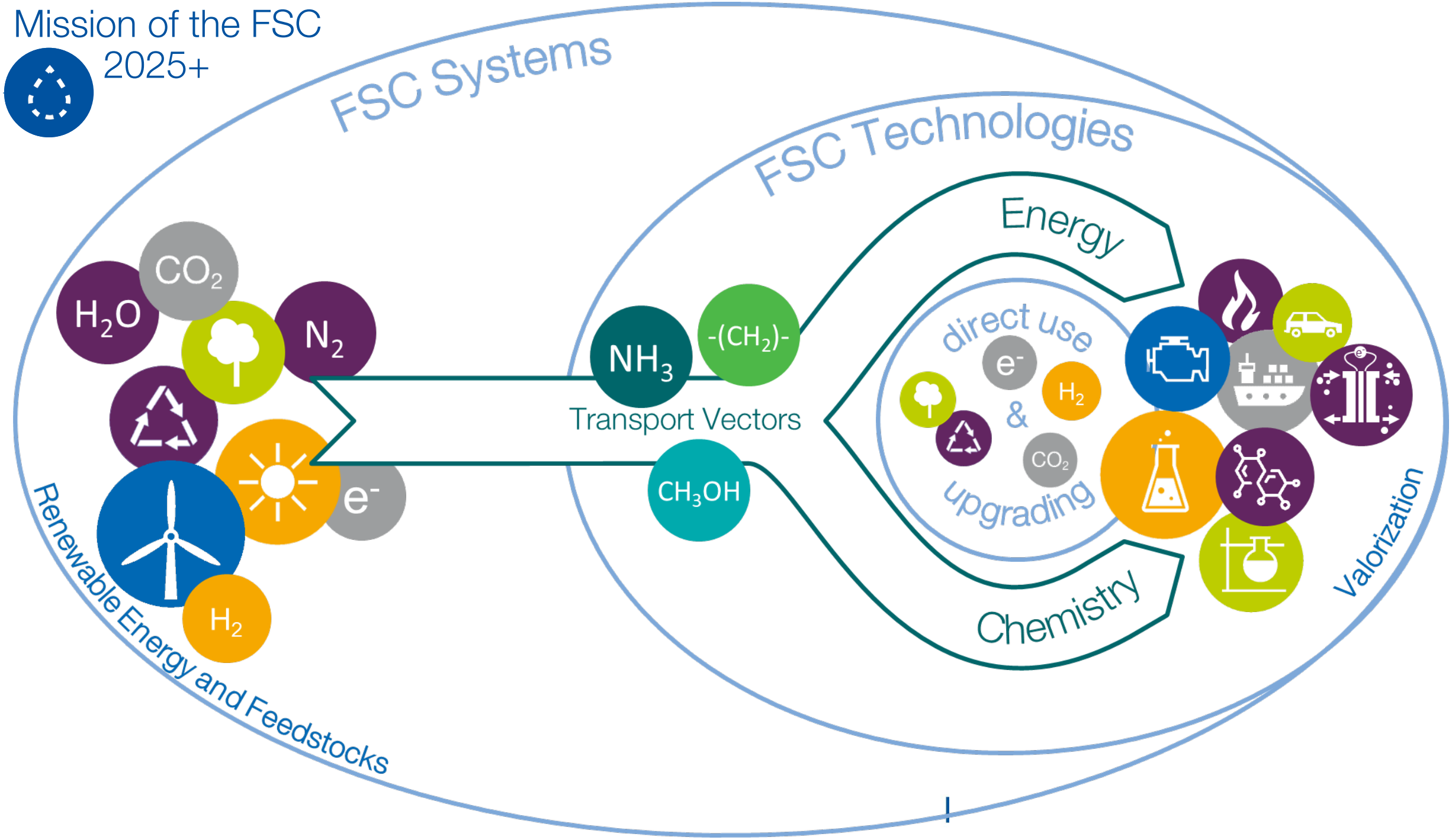


Produkt	Siedepunkt (°C)	Anteil (%)	
Wasserstoff	- 253	1	
Methan	- 161	16	
Ethen	- 104	34	**Ethen**
Ethan	- 87	2	
Propen	- 47	17	**Propen**
Propan	- 42	1	
C_4-Schnitt :		10	
Isobuten	- 6,9		**Buten/ Butadiene**
1-Buten	- 6,3		
Butadien	- 4,4		
Pyrolyse-benzin :		19	
Isopren	+ 34		
Benzol	+ 80		**BTX (Aromatics)**
Toluol	+ 110		
p-Xylol	+ 138		



FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Mission of the FSC 2025+



Integration of Feedstocks and Energy Sources

Bio-hybrid Fuels

reactive	reactive	unreactive
C-O, C-N functionality	bifunctional molecules	C-O, C-N functionalities
Chemical Building Blocks	**Monomers**	**Solvents**

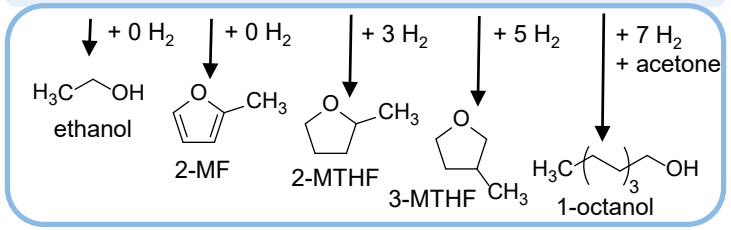
https://pubs.acs.org/doi/10.1021/acs.chemrev.7b00571v

Biofuels

Bio-based Intermediates

Lignocellulosic Biomass

Platform Molecules



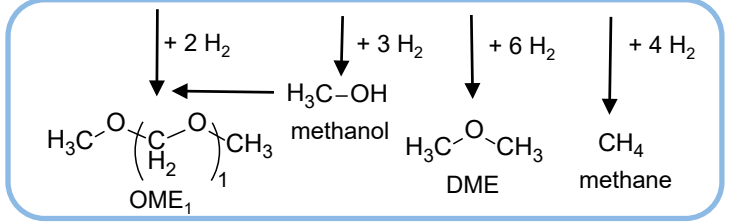
ReConvert

Energy Carriers

Recycling-based Platform Molecules

to be discusses

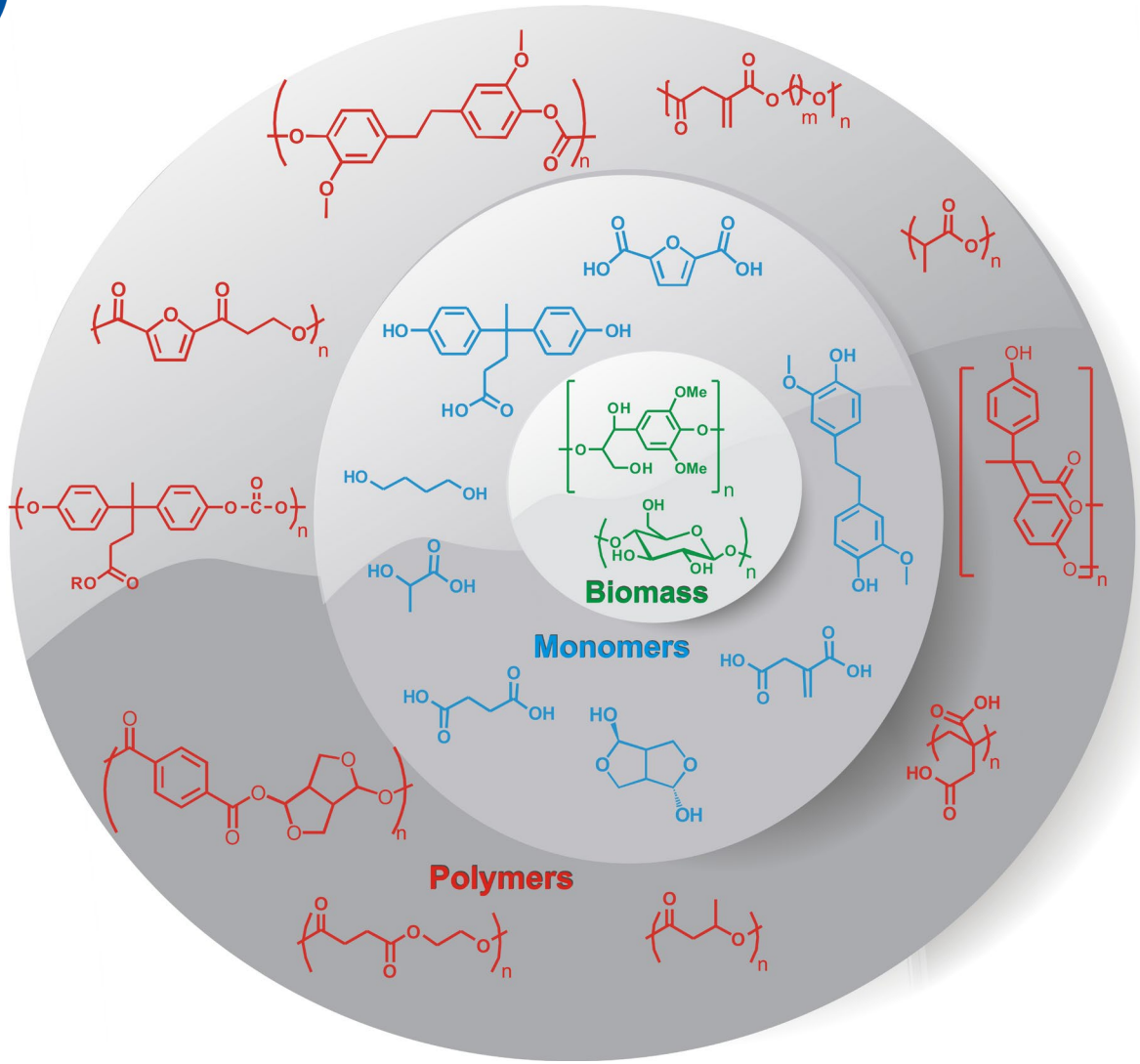
Carbon Dioxide



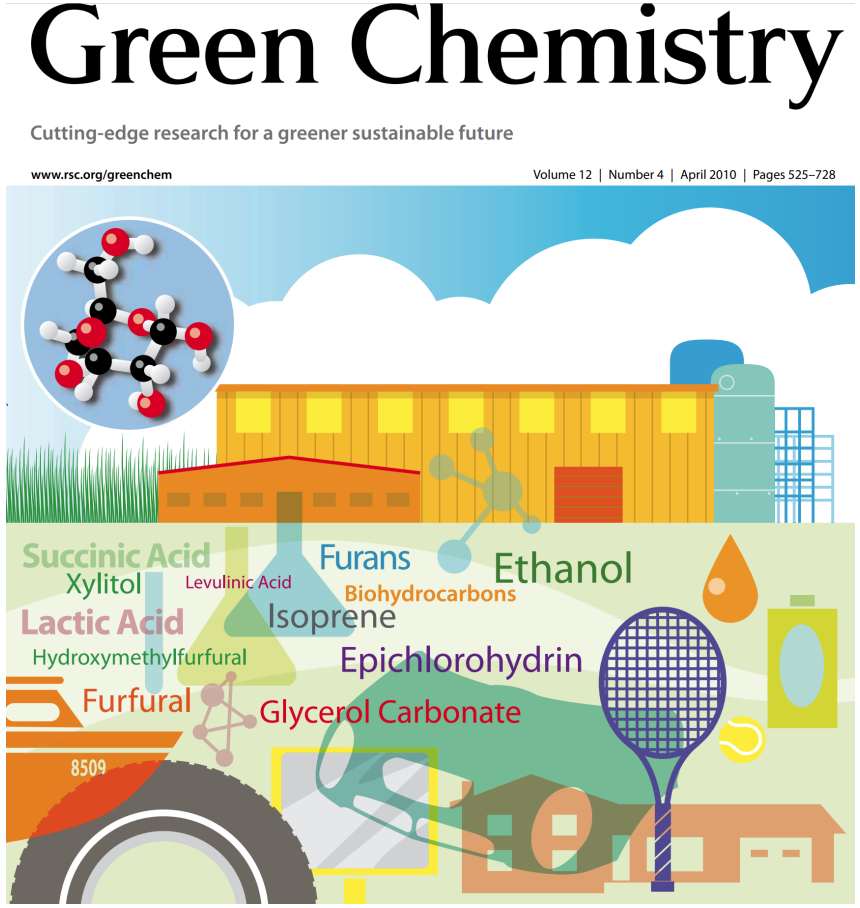
E-Fuels

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Valorising the diversity of biomass



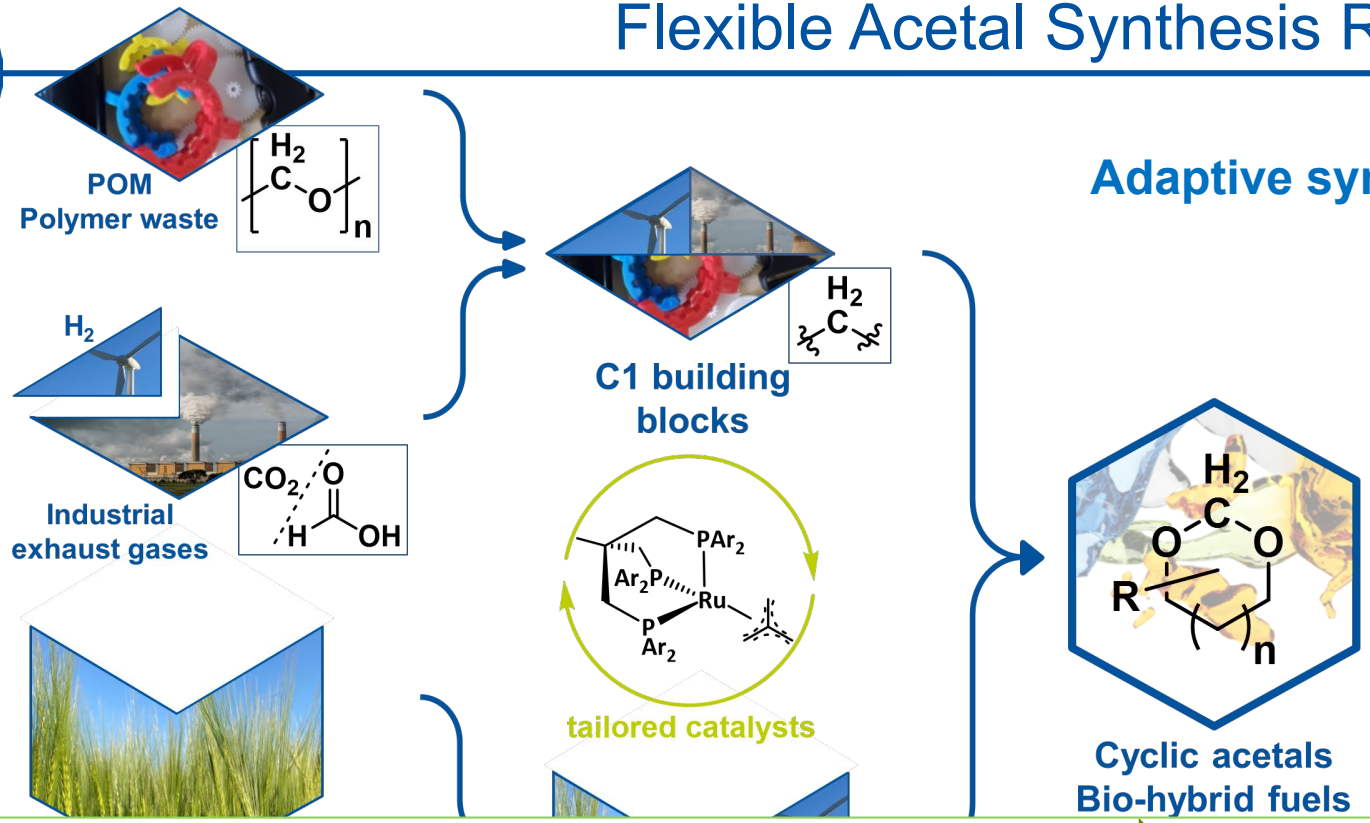
I. Delidovich, P. J. C. Hausoul, L. Deng,
R. Pfützenreuter, M. Rose, R. Palkovits, *Chem. Rev.* **2016**, 116 (3), 1540-1599



J. J. Bozell & G. R. Petersen, *Green Chem.* **2010**, 12, 539

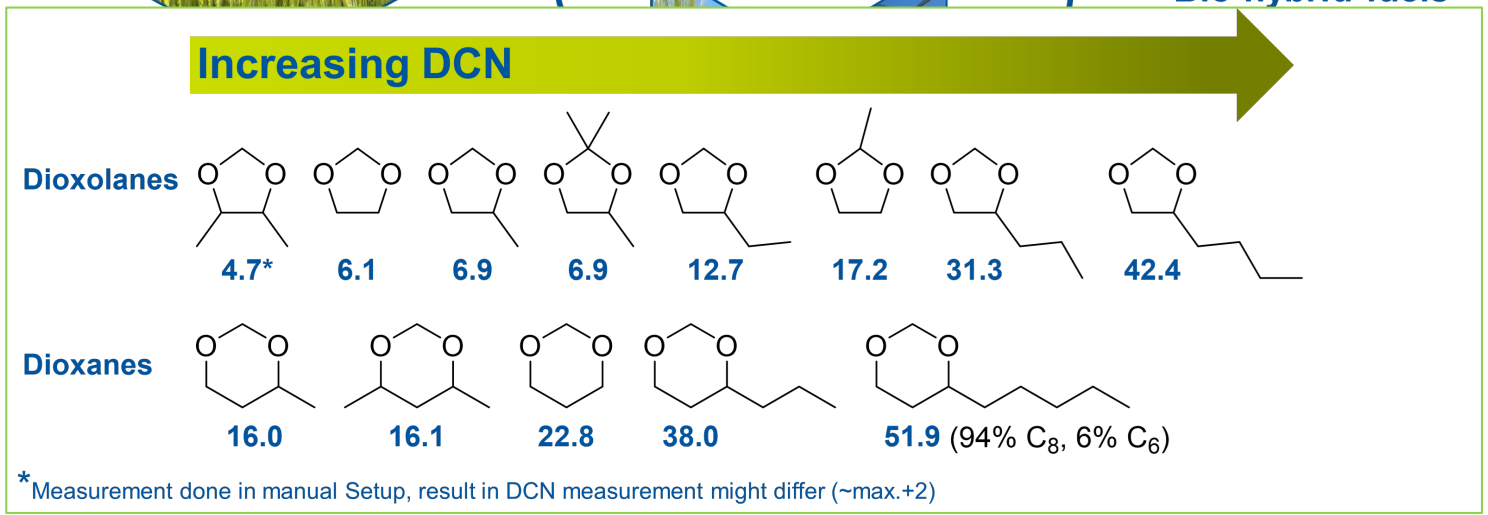
FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Flexible Acetal Synthesis Routes



Adaptive synthesis route to bio-hybride fuels:

- C-sources can be switched: biomass, polymer waste & industrial exhaust gases
- Adaptation to regional and seasonal availabilty

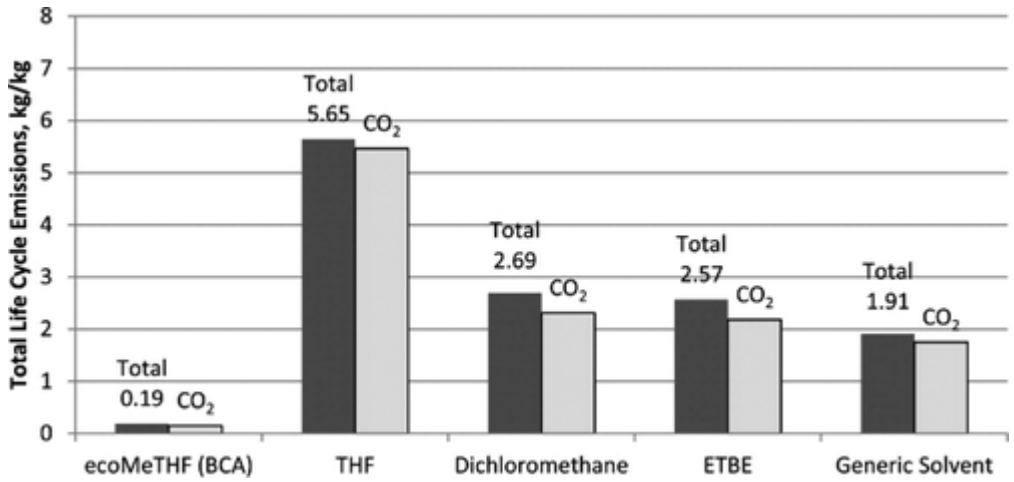


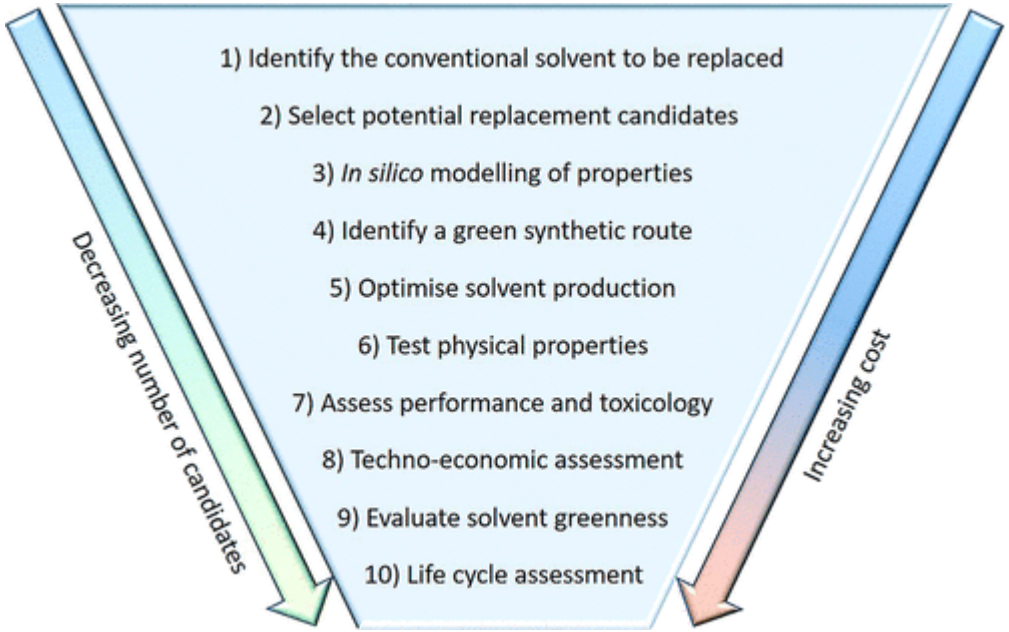
*Measurement done in manual Setup, result in DCN measurement might differ (~max.+2)

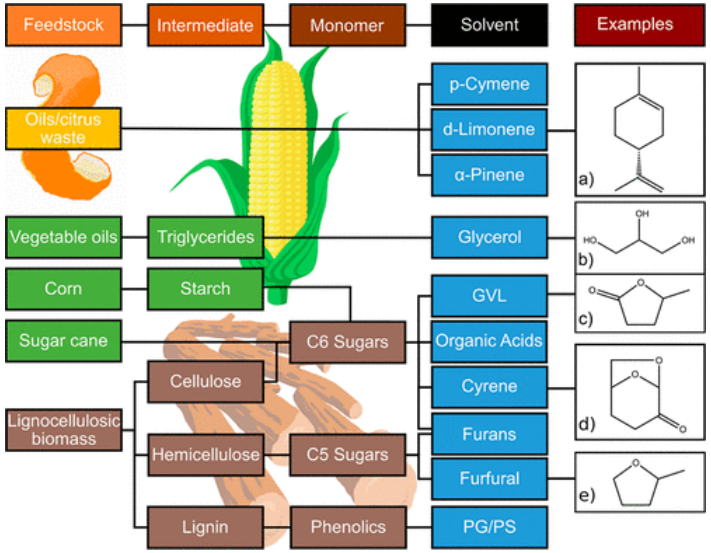
J. Klankermayer, K. Beydoun, K. Thenert, J. Wiesenthal, C. Hoppe, *ChemCatChem* **2020**, *12*, 1944-1947.
K. Beydoun, J. Klankermayer, *ChemSusChem* **2020**, *13*, 488-492
S. Westhues, J. Idel, J. Klankermayer, *Sci. Adv.* **2018**, *4*, eaat9669.
EN 17155

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Green Solvents







https://pubs.acs.org/doi/10.1021/acs.chemrev.7b00571

Green Solvents

Environmental, health and safety assessment of organic solvents

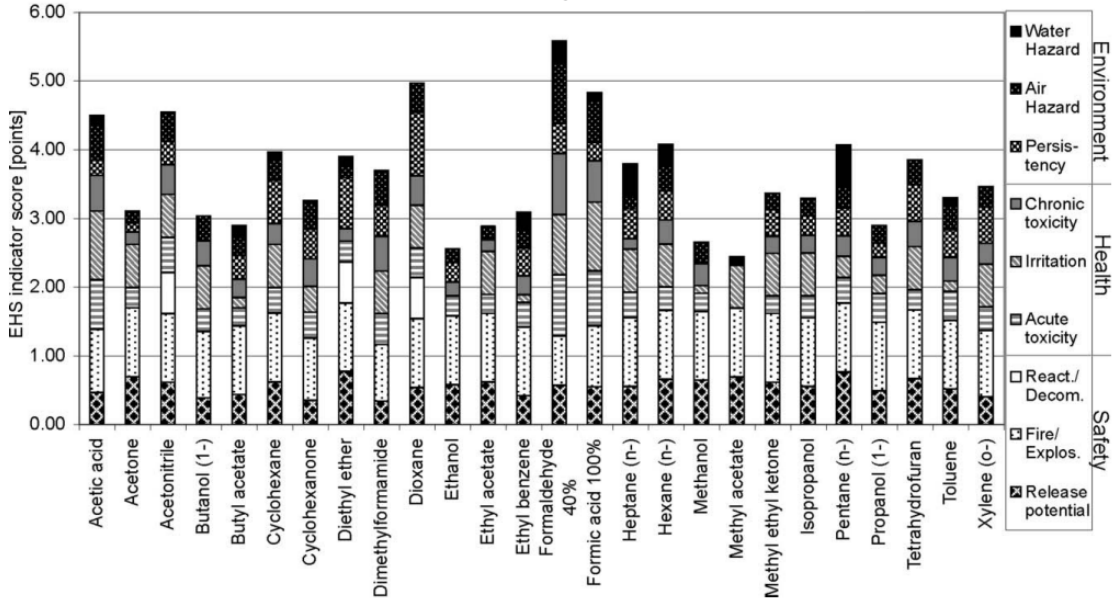


Fig. 2 Results of the EHS method for the 26 pure organic solvents (step (1) in the framework for the assessment of green solvents). The EHS result score is composed of environmental indicators (water and air hazard, persistency), as well as indicators for health (chronic and acute toxicity and irritation) and safety (reaction/decomposition, fire/explosion, release potential) hazards. The results were calculated using the EHS-Tool.[14]

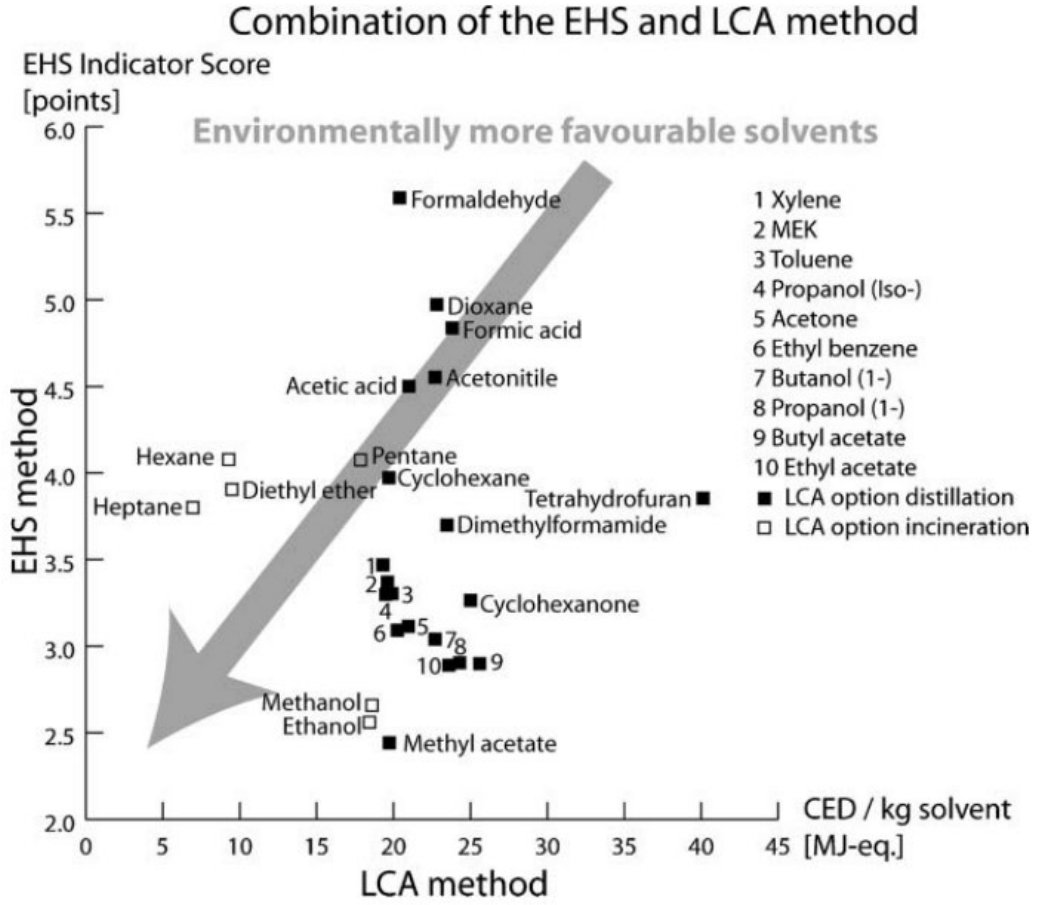


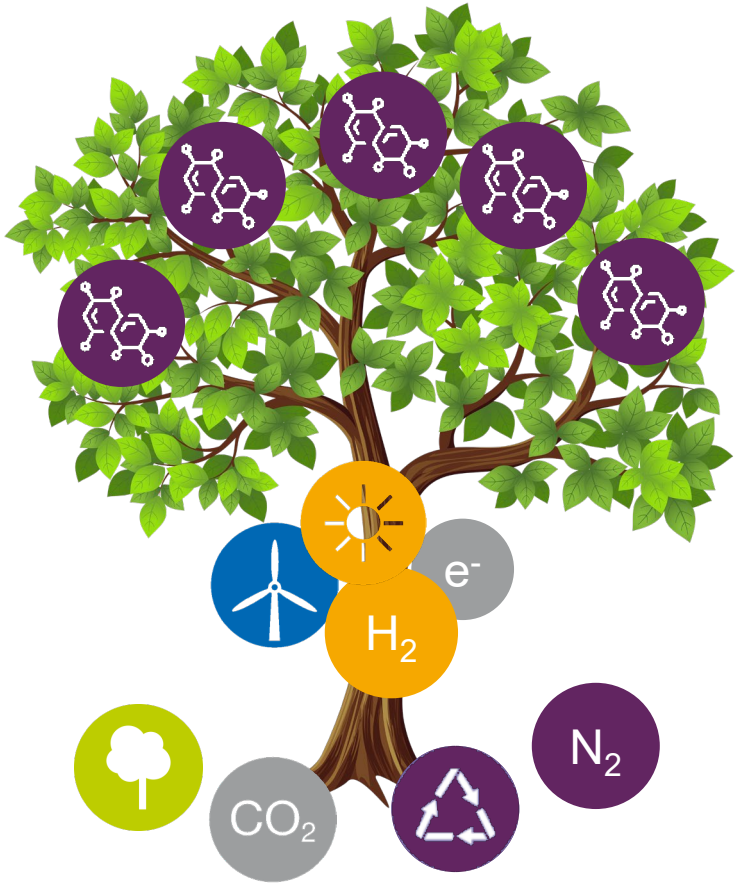
Fig. 4 Environmental assessment of the 26 organic solvents: combination of the EHS method with the LCA method (step (3) of the framework for the assessment of green solvents).

https://pubs.rsc.org/en/content/articlepdf/2007/gc/b617536h

Workshop Results

New Chemist-Tree

based on
Chemical energy carriers, biomass, CO_2, recycling



Targets:

1. Better paths to known products

2. Better performance of novel products
   → integrated product and process design

Measures of „performance“

- Properties for Application
- Recycability via selective bond cleavage
- Biodegradability
- Overall TCA, toxicology, etc.

Methods:

Adaptivity of transformations regarding feedstock and energy base, etc.…

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

Required Competences

Molecular Modelling & Analysis
- predicting molecular properties, mechanisms, etc.
- using data-intelligent synthetic accessibility
- operando analyses

Leonhard, Kethan, Piccini, Zobel,
de Beer, Schönebeck

Molecular Transformations
- Catalytic bond formation & cleavage
- Different Energy Inputs
- Flexible Feedstock base
- Adaptive Transformations

Blank, Rother, Lauterbach, Magnus, Bolm,
Herres-Pawlis, Leitner, Leonori, Klankermayer,
Palkovits, N.N. Simon, Schwaneberg

Reaction Eng. & Process Design
- Integrated Product & Process Design
- Adaptive Technologies/Multiphase Reactors
- Hybride Processes
- Integrated Value Chains

Jupke, Mitsos, Eichel, Wessling, Mechler
Keller, Linkhorst

System
- Feedstock Availability
- Supply Chain Flexibility/Resielence
- Assessment (LCA and beyond)

Walther, van der Assen, Mitsos

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY

The Fuel Science Center 2025+

Adaptive Conversion Systems for Renewable Energy and Carbon Sources

PI-Workshop | Follow-Up Proposal 2025+

07.06.2023

FSC The Fuel Science Center | RWTH AACHEN UNIVERSITY