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UNITÉ DE CATALYSE ET CHIMIE DU SOLIDE

Transforming CO_2 - Selected examples of hydrogenation pathways to olefins and oxygenates

Andrei Khodakov, CNRS

CNRS Research Director

Unit of Catalysis and Chemistry of Solids (UCCS)

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UNIT OF CATALYSIS AND CHEMISTRY OF SOLIDS (UCCS), FRANCE

UCCS is a joint Laboratory of University of Lille, Centre National de la Recherche Scientifique (CNRS), Centrale Lille Institute, University of Artois

- Staff: 137 (104 researchers, 33 technical staff)
  + 6 Professors Emeritus
- Students: 80 Ph.D.
- Postdocs: > 20

- *>200* publications/year in international peer-reviewed journals
- >200 communications/year

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CATSUSCHEM (SUSCAT) TEAM
Sustainable Catalysis

Thermo and Photo Reactors

High throughput reactors

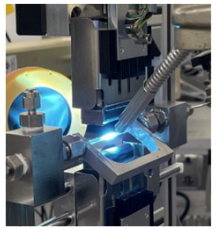
Catalyst and process design for C_1 chemistry

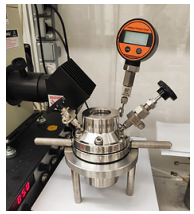
CO_2, CO, methane, methanol, formaldehyde and formic acid

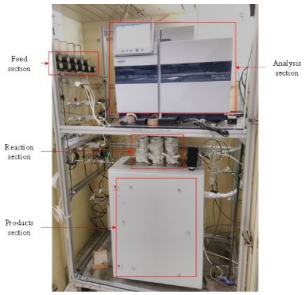
Our focus: Reactivity in thermo- and photocatalysis under mild conditions

RESEARCH TOPICS:

– **CO_2 upgrading** (hydrogenation, reduction);
– **Methanol-mediated hydrocarbon synthesis from CO and CO_2;**
– **Fischer-Tropsch synthesis from CO and CO_2;**
– **Synthesis of methanol and dimethyl ether;**
– **Methane activation** (methane coupling, partial oxidation, reforming).







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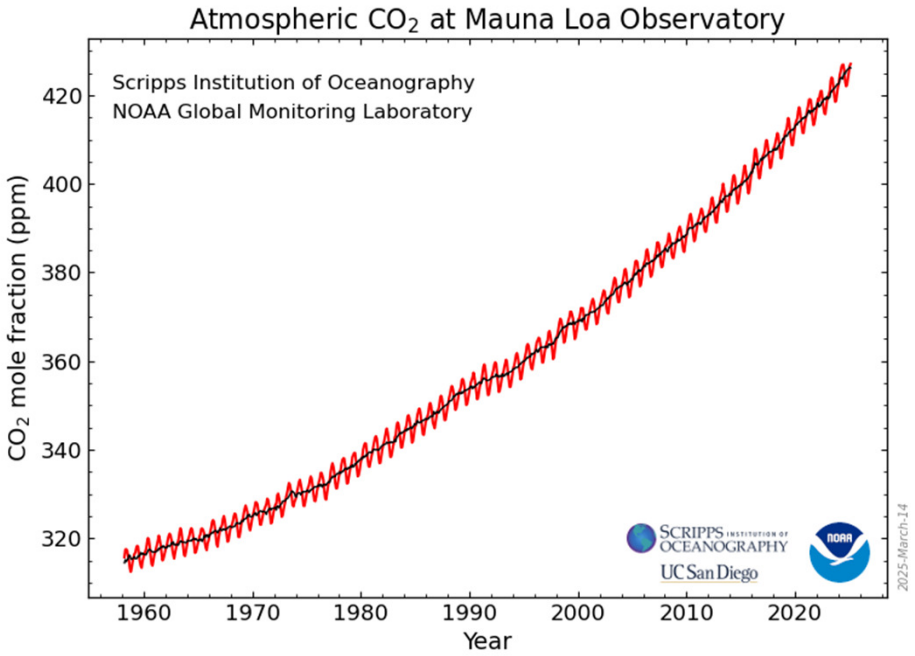
FACTS & NUMBERS

Enviromental motivation



March 2025: 427.09 ppm
June 2023: 423.68 ppm
Last updated: March 14, 2025

https://gml.noaa.gov/ccgg/trends/

FACTS & NUMBERS

Economic motivation

EU carbon price has rocketed from 10 € to 70-100 €

European Union Carbon Permit allows the holder to emit one ton of CO_2 or CO_2 equivalent greenhouse gas.

ENERGY TRANSITION

Tools

Shift to Renewable Feedstocks

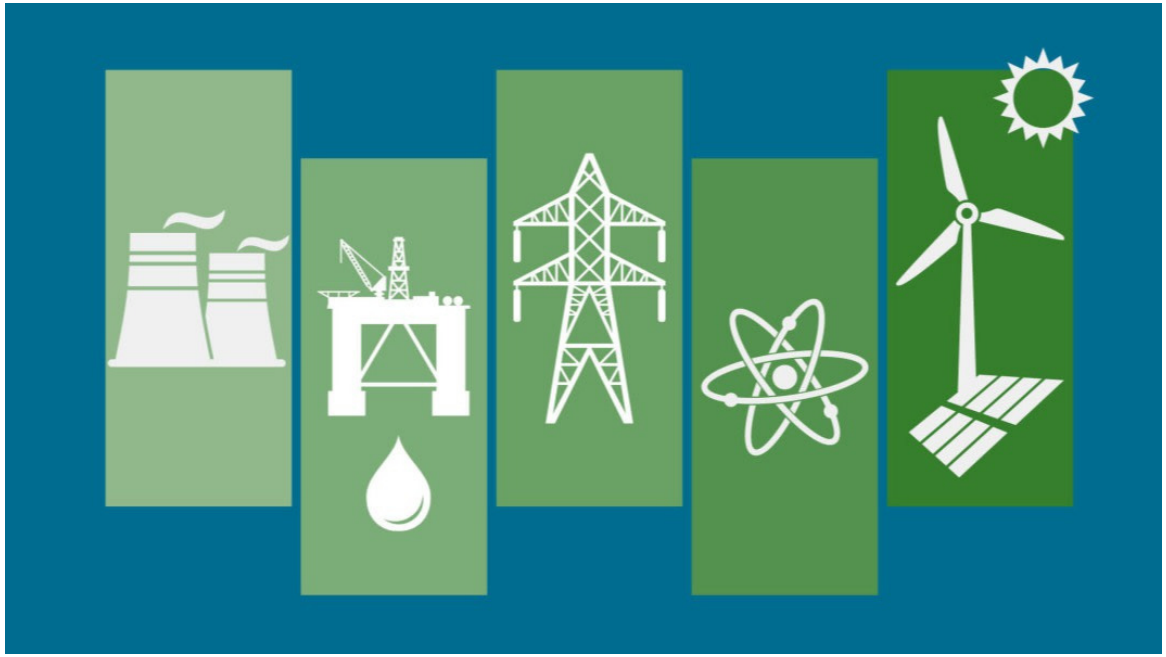
Shift to Renewable Energy

Process Efficiency

Circularity

Carbon Capture & Storage

Carbon Capture & Utilisation



https://www.ft.com/reports/energy-transition-guide

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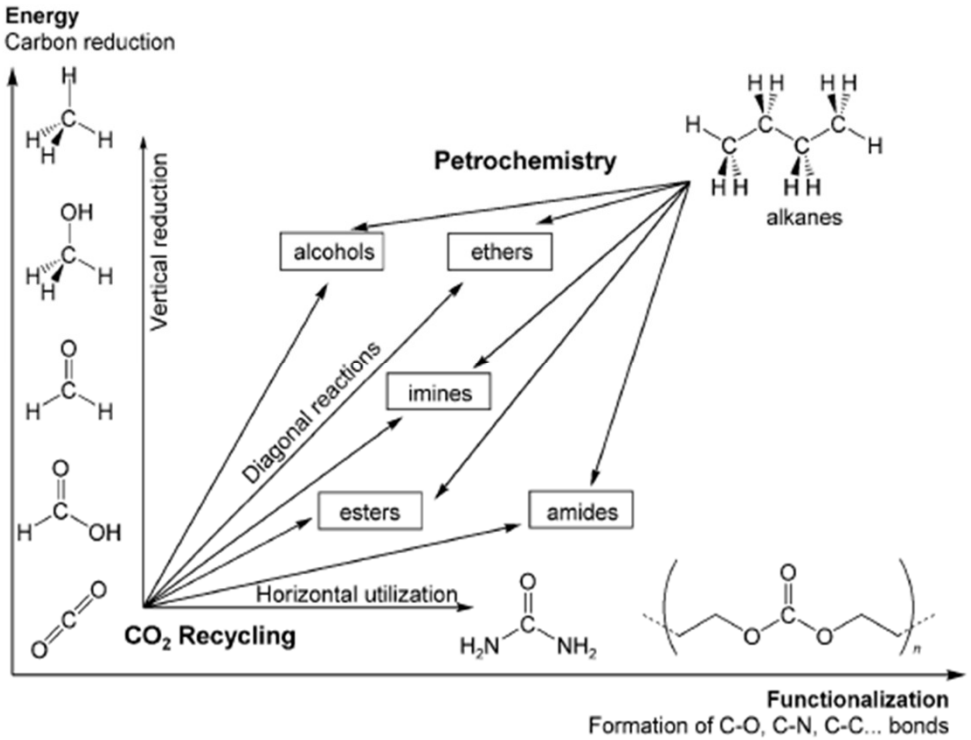
Transforming CO_2: Thermodynamic aspects

Energy versus functionalization



Carbon dioxide has a low energetic level and thus a high thermodynamic stability.

$(\Delta_f H_o) = -394$ kJ/mol

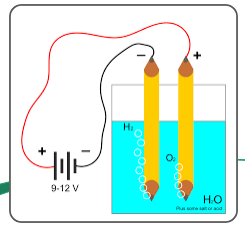
"Horizontal approach" to low energy products

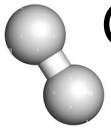
"Vertical approach" to high energy products

Angew. Chem. Int. Ed. 2012, 51, 187 –190

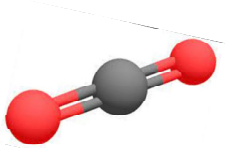
CO_2 REDUCTIVE CHEMICAL CONVERSION

Two steps CO_2 reductive conversion





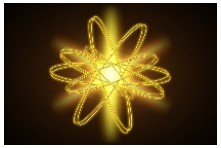
Green hydrogen, Hydrogenation



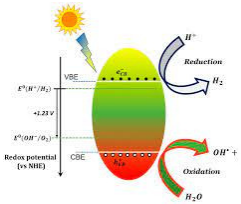
Advantages of two steps CO_2 conversion

Higher productivity

Higher maturity



Single step CO_2 reductive conversion



Electrocatalysis

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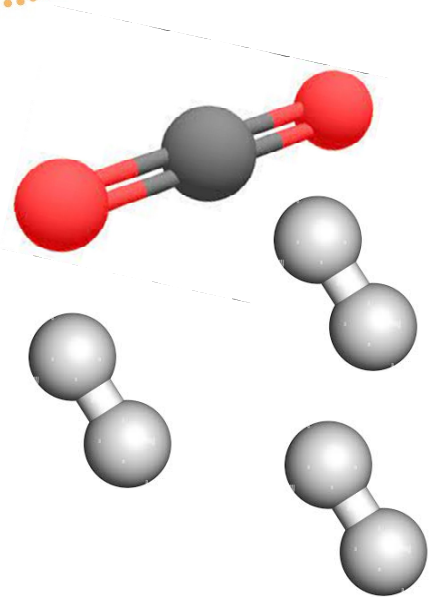
CO_2 HYDROGENATION



H_2/CO Syngas

Methane

Methanol

Formates

Dimethyl Ether (DME)

Light Olefins

Thermodynamics & Kinetics

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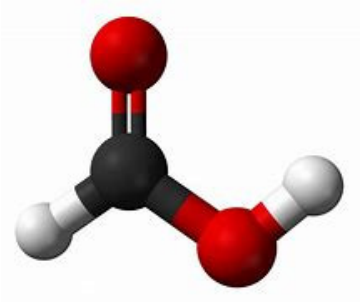
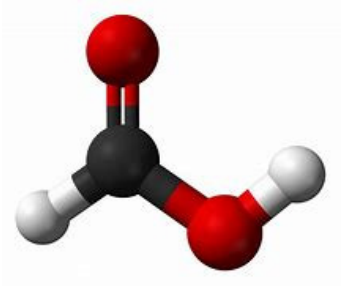
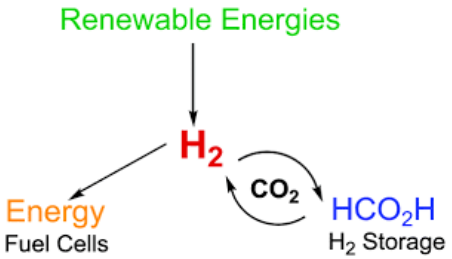
FORMATES



CO_2 HYDROGENATION TO FORMIC ACID





Reaction is entropically disfavored,

			ΔG° (kJ mol^{-1})	ΔH° (kJ mol^{-1})	ΔS° (J mol^{-1} K^{-1})
CO_2 (g)	+ H_2 (g)	$\rightleftharpoons$ HCO_2H (l)	32.9	-31.2	-216

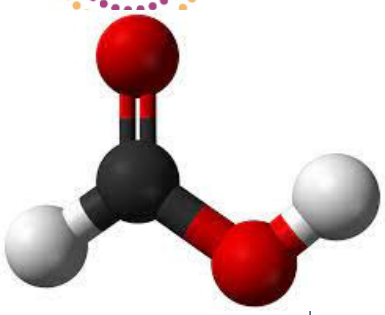
Thermodynamic equilibrium has to be disturbed by secondary reaction or molecular interaction:

Hydrogen storage material in the energy industries
Antibacterial agent
Insecticide
De-icing agent in various
Major role in synthetic chemistry as an acid, a reductant and a precursor for syntheses.
Promising fuel source in direct liquid fuel cell systems
Feed for microorganisms

How to improve thermodynamics?

Esterification
Neutralization with a weak base such as tertiary amines or alkali/alkaline earth bicarbonates.

FORMIC ACID: CURRENT TECHNOLOGY



HCOOH

$$CH_3OH + CO \rightarrow HCOOCH_3$$

40 atm, 80 ℃, alkaline solution

Direct hydrolysis

$$HCOOCH_3 + H_2O \rightarrow HCOOH + CH_3OH$$

Formamide hydrolysis

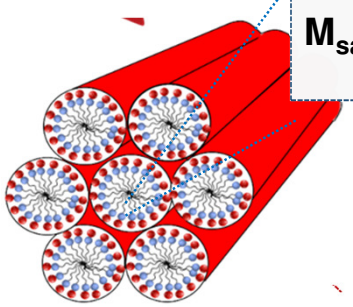
$$HCOOCH_3 + NH_3 \rightarrow HCONH_2 + CH_3OH$$

$$HCONH_2 + H_2O + 1/2H_2SO_2 \rightarrow HCOOH + ½(NH_4)_2SO_4$$

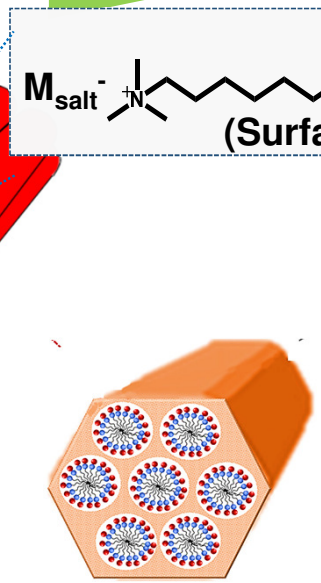
Multistep process
Significant Capital & Energy intensity

SOLID MICELLAR CATALYSTS

Proposed Strategy

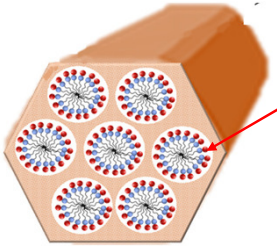


Micellar



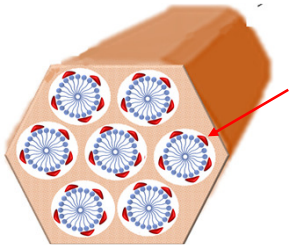
SOMIC

Possible Structures



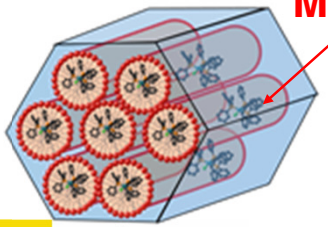
Single Sites

Single Site SOMIC



Clusters or Particles

Clusters/Particles SOMIC



Metal complex

Metal Complex SOMIC

Cetyltrimethyl ammonium bromide (CTAB)

*Appl. Catal. B, 290 (**2021**) 120036*

*Appl. Catal. B, (**2021**): 120730*

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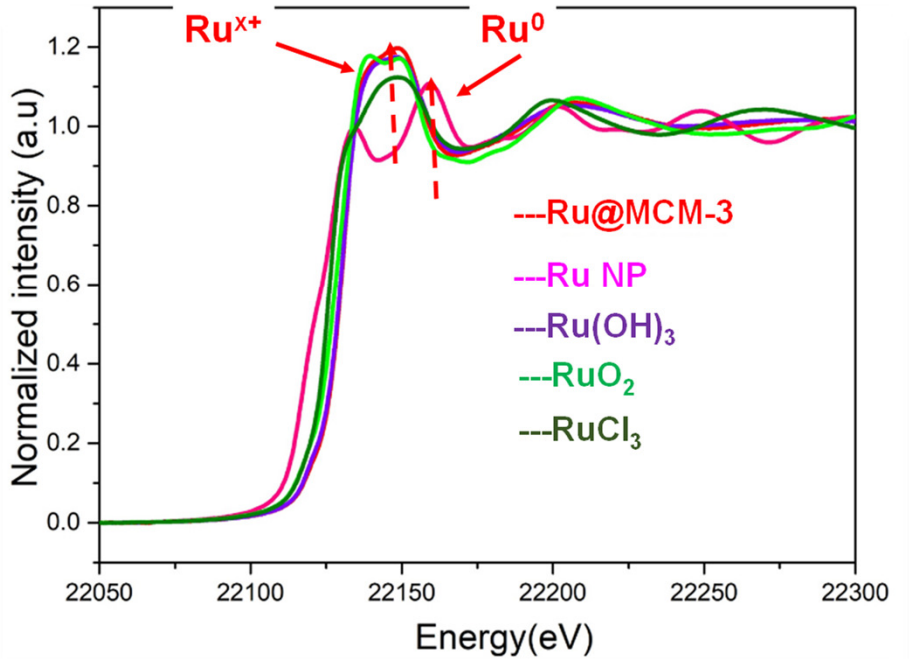
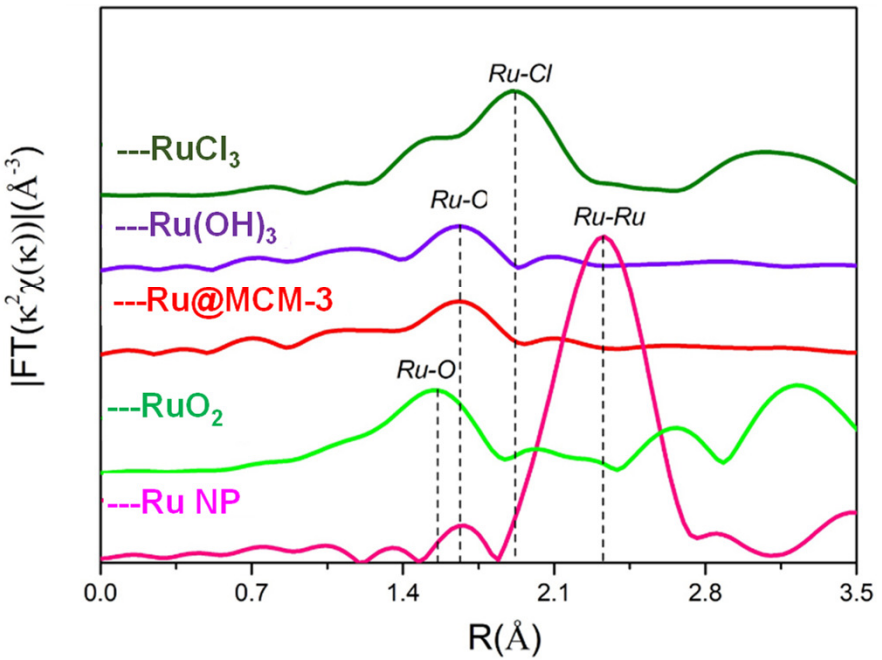
Ru Single Site SOMIC

Characterizations: Structure of Ru (XANES)

The spectra of Ru K-edge XANES



The spectra of Ru K-edge FT EXAFS

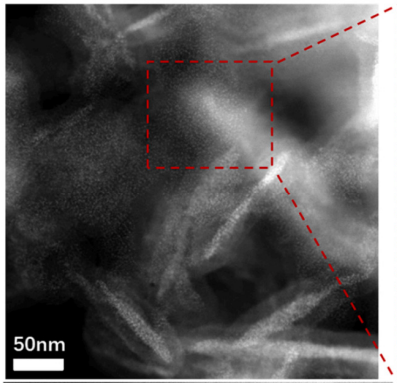


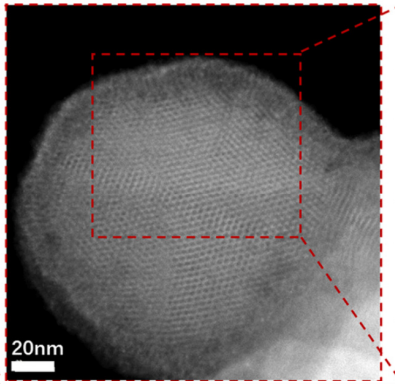
- The results of XANES and EXAFS both shown the Ru in the Ru@MCM is oxidation, not Ru metal, which indicate Ru is single site in the Ru@MCM.

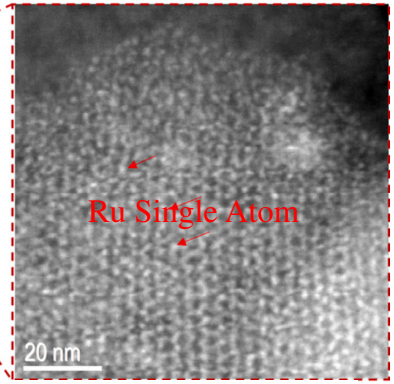
Appl. Catal. B: Environ. 277 (2020) 119

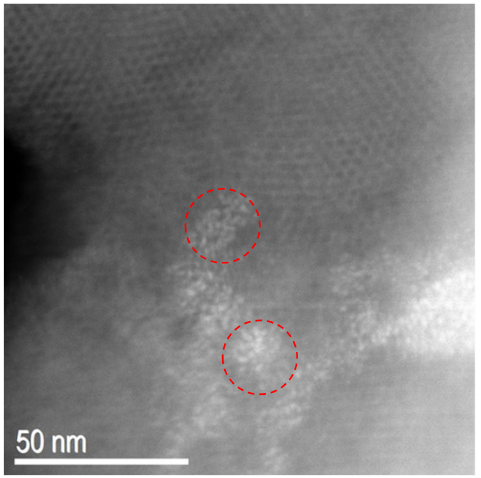
Ru Single Site SOMIC

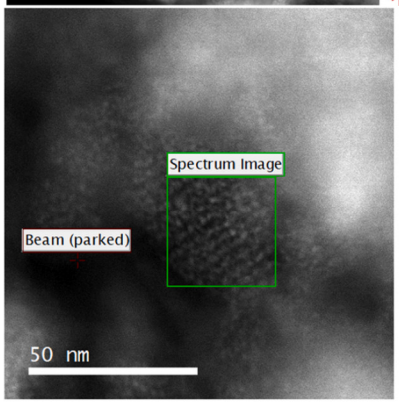
Characterizations: Morphology Structure (TEM)

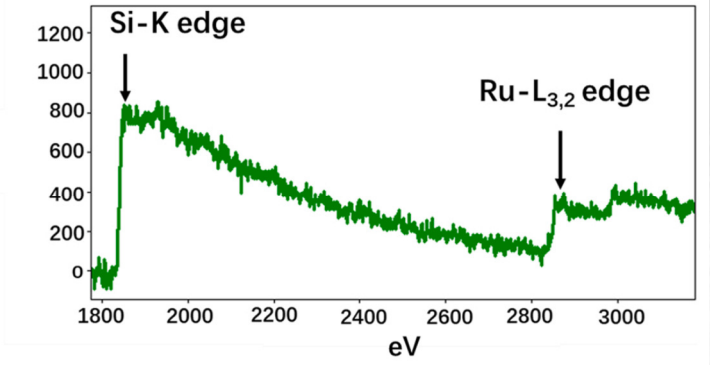


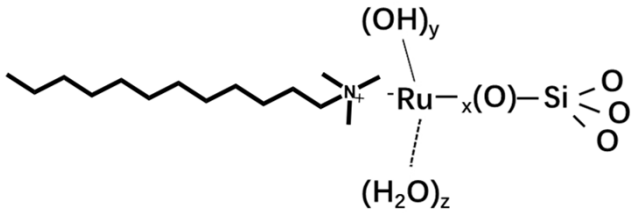












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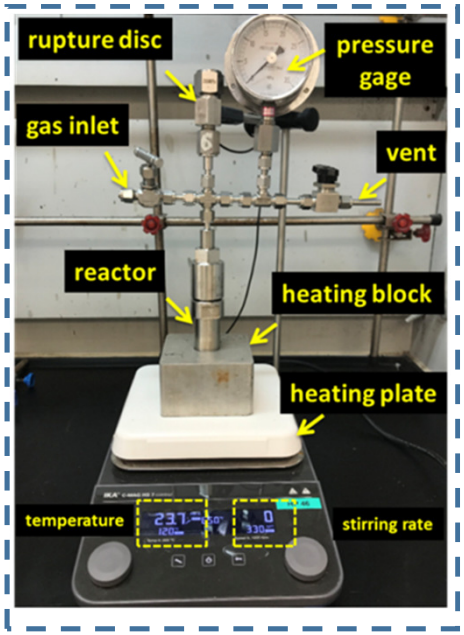
Ru Single Site SOMIC

$CO_2 + H_2$ —(TEA)→ $HCOO^- {}^+HN\text{-}(CH_2\text{-}CH_3)_3$

(TEA)

Reaction System



NMR

***Typical Reaction conditions**: 0.32 mg Ru; 0.9 g TEA, 6 g water or no water, CO_2 3 MPa, H_2 2 MPa, 90 °C*

Catalyst System

Catalyst:	References:
Ru@MCM-1	Ru@MCM-NH_4^+
Ru@MCM-3	Ru/MCM
Ru@MCM-5	Ru/C (commercial)
	$RuCl_3$
	$Ru(OH)_3$

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Literatures

Catalysts	Solvent	Temp. /°C	Base	p(H_2/CO_2) /MPa	Time /h	Con. /mol*L^{-1}	TON	TOF /h^{-1}
Ru@MCM-41	**Water**	**110**	**NEt_3**	**2/3**	**15**	**1.2**	**2729**	**182**
Ru@MCM-41	**-**	**90**	**NEt_3**	**2/3**	**15**	**4.0**	**1582**	**105**
Ru/LDH	D_2O	100	NaOH	1/1	24	-	698	29
RuFe Nanoparticles	D_2O/DMSO	60	IL	1/2	17	0.01	400	24
[Ru_1]@UiO-66	D_2O/DMSO 1.8:36.4 mol%	27	DMF/DBU	1.2/0.3	0.5	-	$3*10^5$	$6*10^5$
[Ru_2]Cl	Water	120	NEt_3	4/4	3	1.79	2150	716
Pd@Ag/TiO_2	Water	100	$NaHCO_3$	1/1	24	0.23	2496	104
Au NP/Al_2O_3	EtOH	70	NEt_3	2/2	20	0.22	215	10
Pd/mpg-C_3N_4	D_2O	150	NEt_3	2.7/1.3	24	0.12	-	-
IrPN/SBA-15	Water	60	NEt_3	2/2	20	0.27	2700	140
Ir(III)/COFs	Water	120	NEt_3	4/4	10	-	6400	1500

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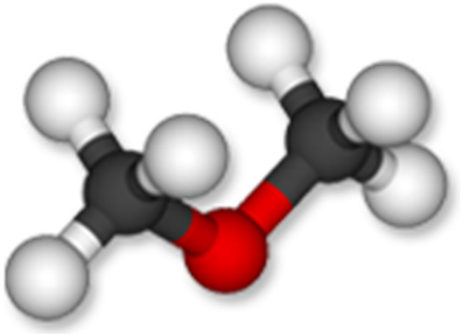
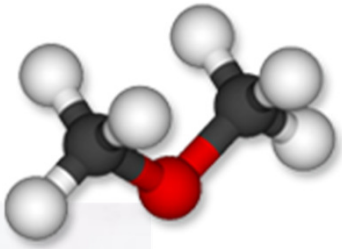
DIMETHYL ETHER



POWER-TO-GAS: DIMETHYL ETHER (DME)



Opportunities of DME as a “carbon neutral“ fuel

-Can be used in conventional diesel engines with a modified fuel injection
-Large potential market
-High cetane number
-Quiet combustion
-Clean burning (soot less – no smoke or particulates)
-LPG-like distribution infrastructure
-100% SO_x reduction

BioDME plant with DME log truck in foreground © *Chemrec*

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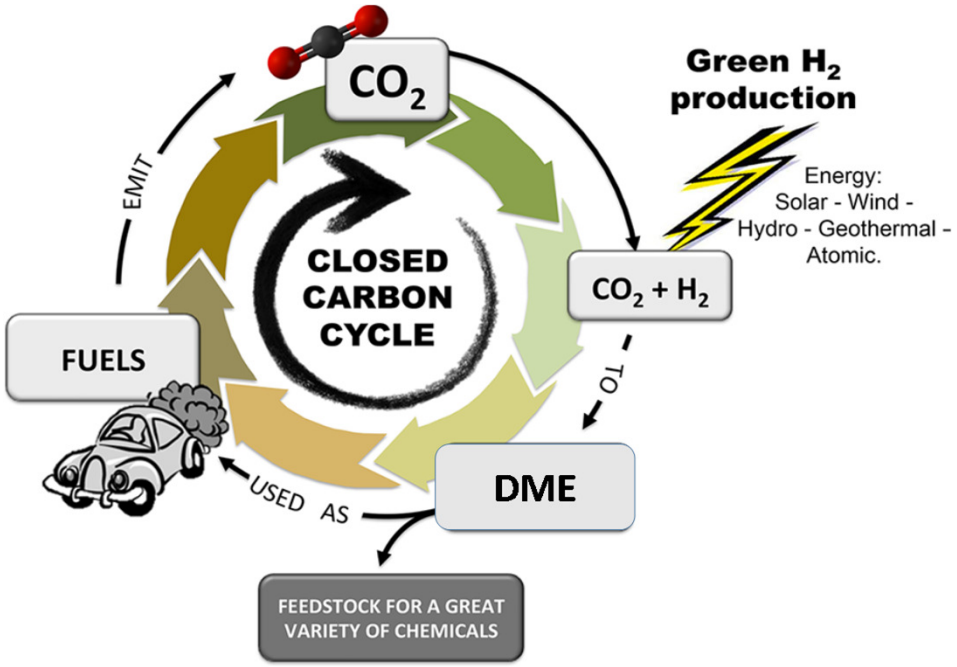
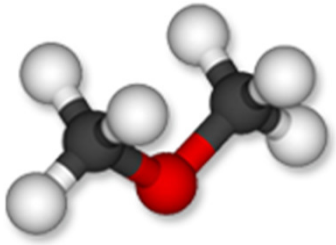
CO_2 HYDROGENATION TO DIMETHYL ETHER





Major and Minor Reactions:

$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$ $\quad \Delta H^0_{273}$=-49.5 kJ/mol

$CO + 2H_2 \leftrightarrow CH_3OH$ $\quad \Delta H^0_{273}$= −90.5 kJ/mol

$2\ CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$ $\quad \Delta H^0_{273}$=−23.4 kJ/mol

$CO_2 + H_2 \leftrightarrow CO + H_2O$ $\quad \Delta H^0_{273}$=41.2 kJ/mol

Chem. Rev. 2017, 117, 9804−9838

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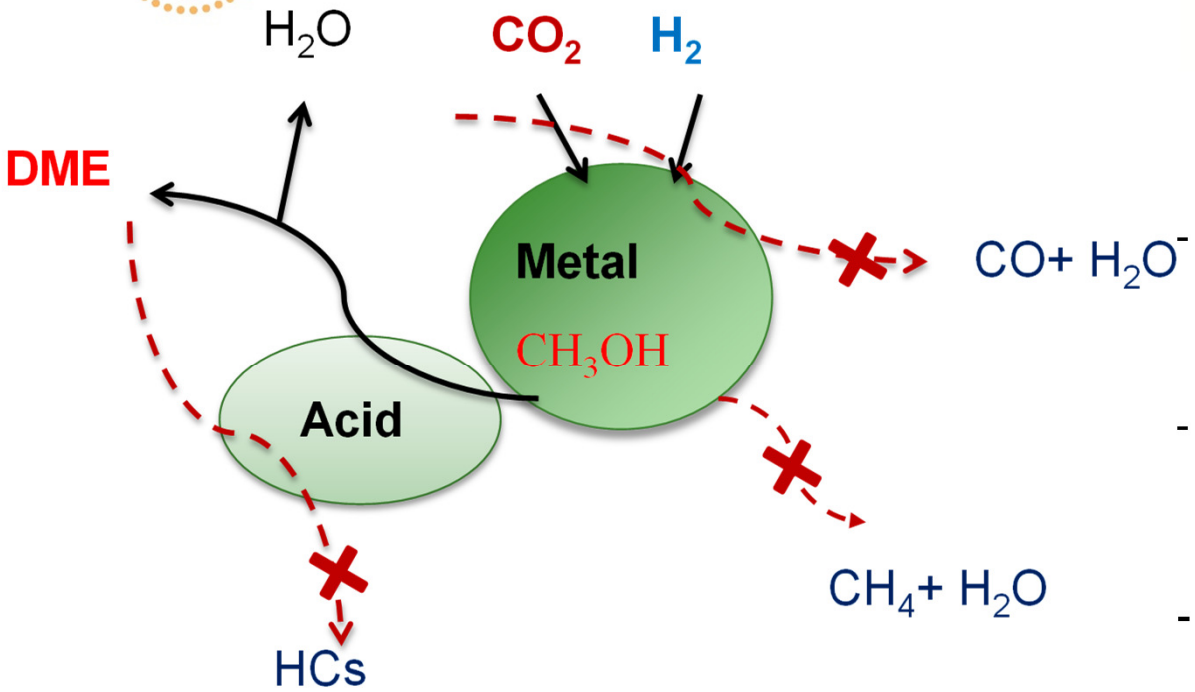
DESIGN OF BIFUNCTIONAL CATALYSTS FOR DME SYNTHESIS



Reverse Water Gas Shift

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

METHANOL SYNTHESIS COMPONENT

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$$

- **ACID COMPONENT FOR DEHYDRATION**

$$2\ CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$$

- INTERACTION BETWEEN TWO COMPONENTS

Interreg 2 Seas Mers Zeeën
e2c
TNO innovation for life
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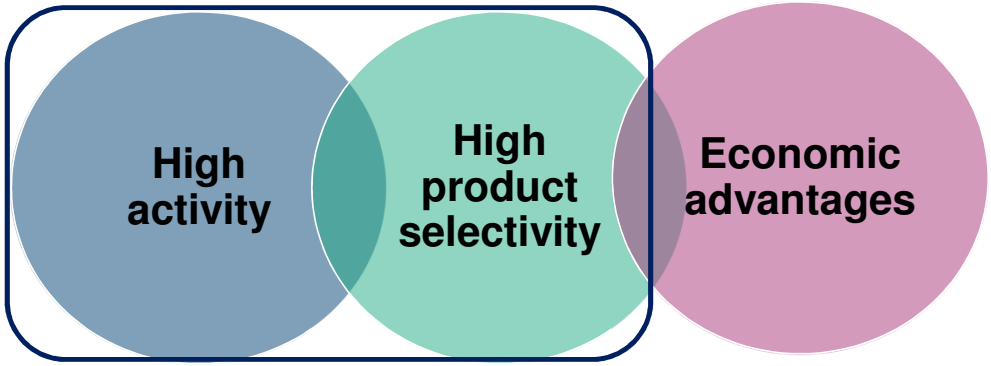
Cu-ZnO SYSTEM: THE MOST STUDIED MATERIAL FOR METHANOL SYNTHESIS



Microstructural characteristics of Cu-ZnO after reduction treatment

High metal (Cu) dispersion (S_{Cu} = 18-23 $m^2 \cdot g^{-1}$ after reduction)

Science **2016**, 352, 969

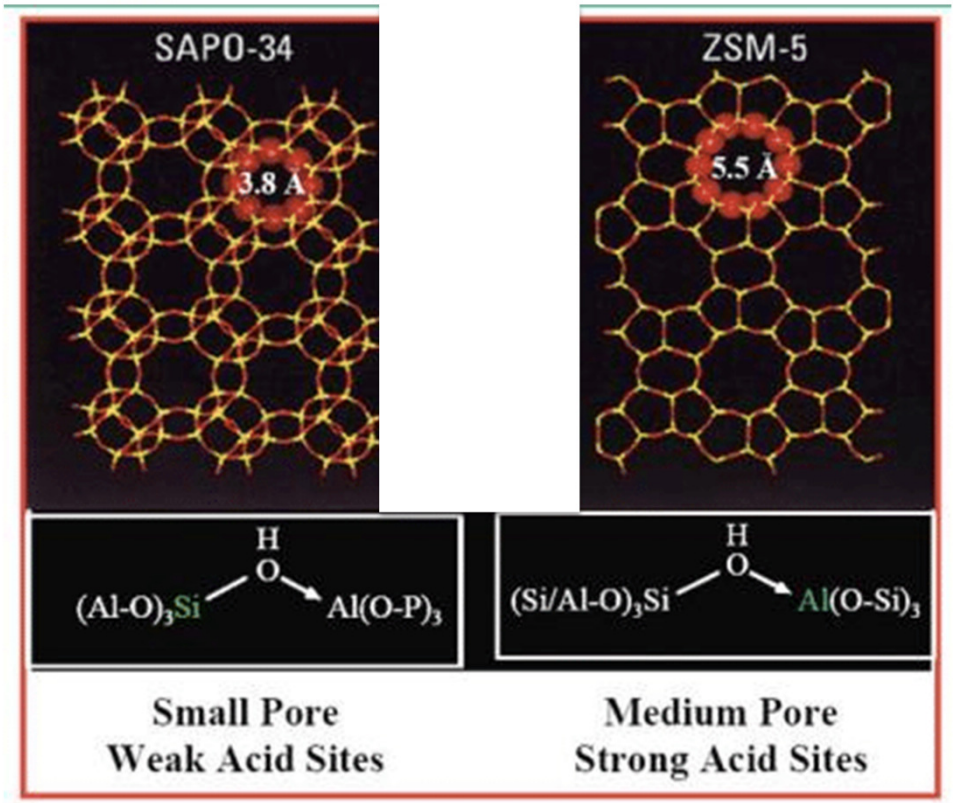
ZnO particles act as spacers between the Cu^0 particles

J. Catal. **2015**, 324, 41

Cu-ZnO synergy: S_{cu} maximized and enhanced Cu-ZnO interaction

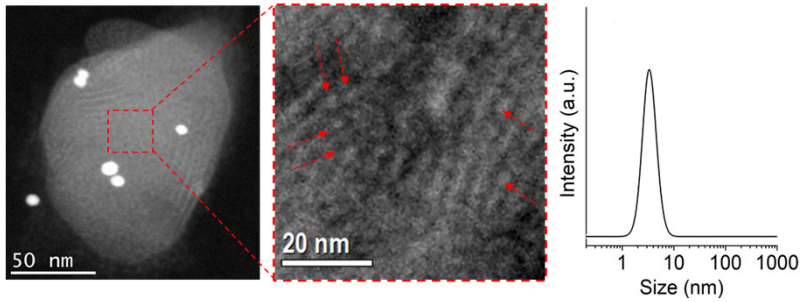
ACID COMPONENT

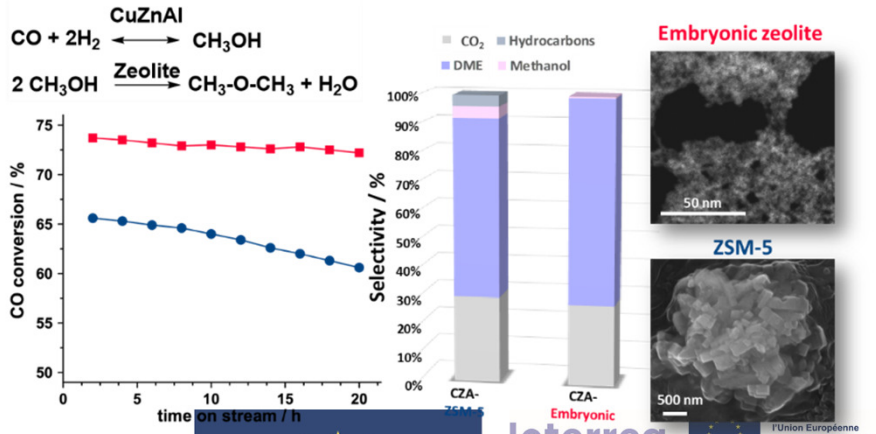
Conventional crystalline zeolites



Embryonic zeolites, weaker than in zeolite but accessible acid sites (coll. with V. Valtchev)

Ana Palčić et al, Micro and Meso Mat. 2021





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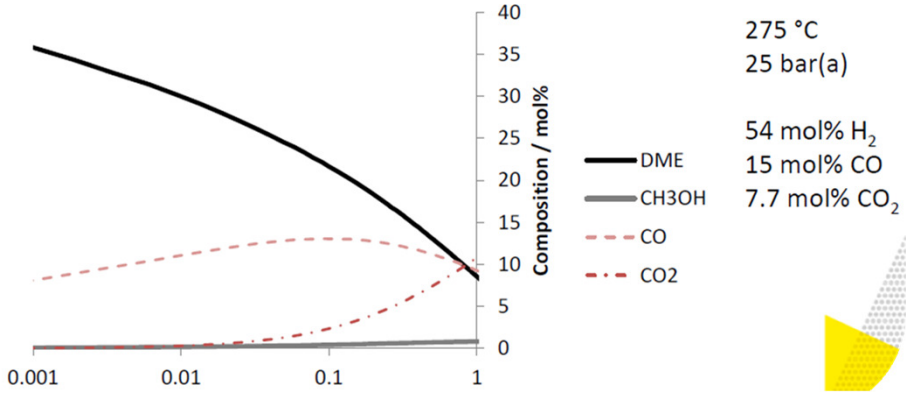
CHALLENGES OF STEADY STATE OPERATION: CO_2 CONVERSION AND DME SELECTIVITY?

SOLUTION: SORPTION ENHANCED DME SYNTHESIS (SEDMES)

TNO

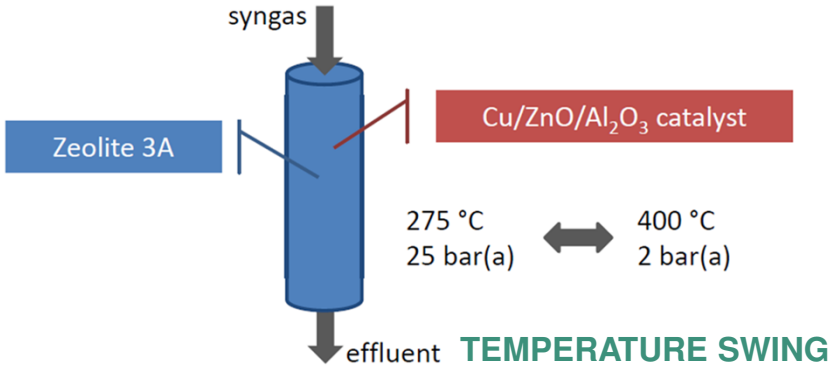
$$2CO_2 + 6H_2 \rightarrow CH_3OCH_3 + 3H_2O$$

Equilibrium with in situ water removal



Residual steam, mol. %

Experimental: sorption enhanced DME synthesis



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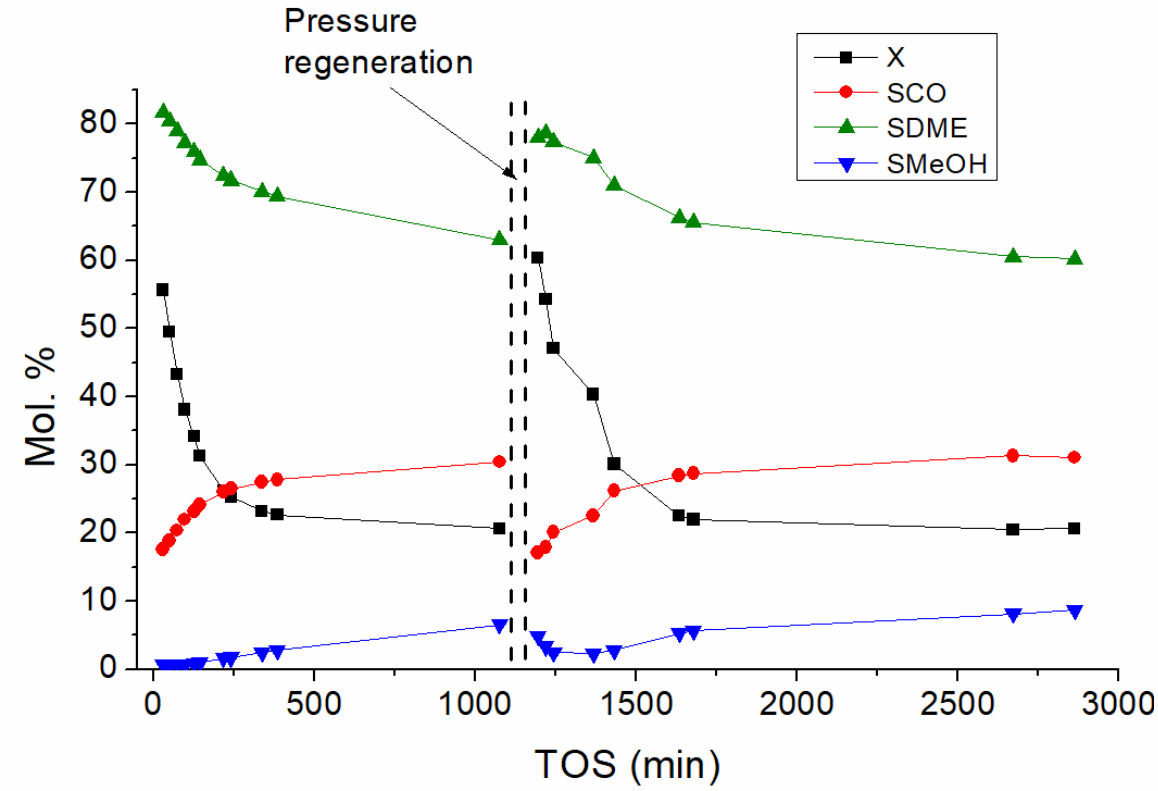
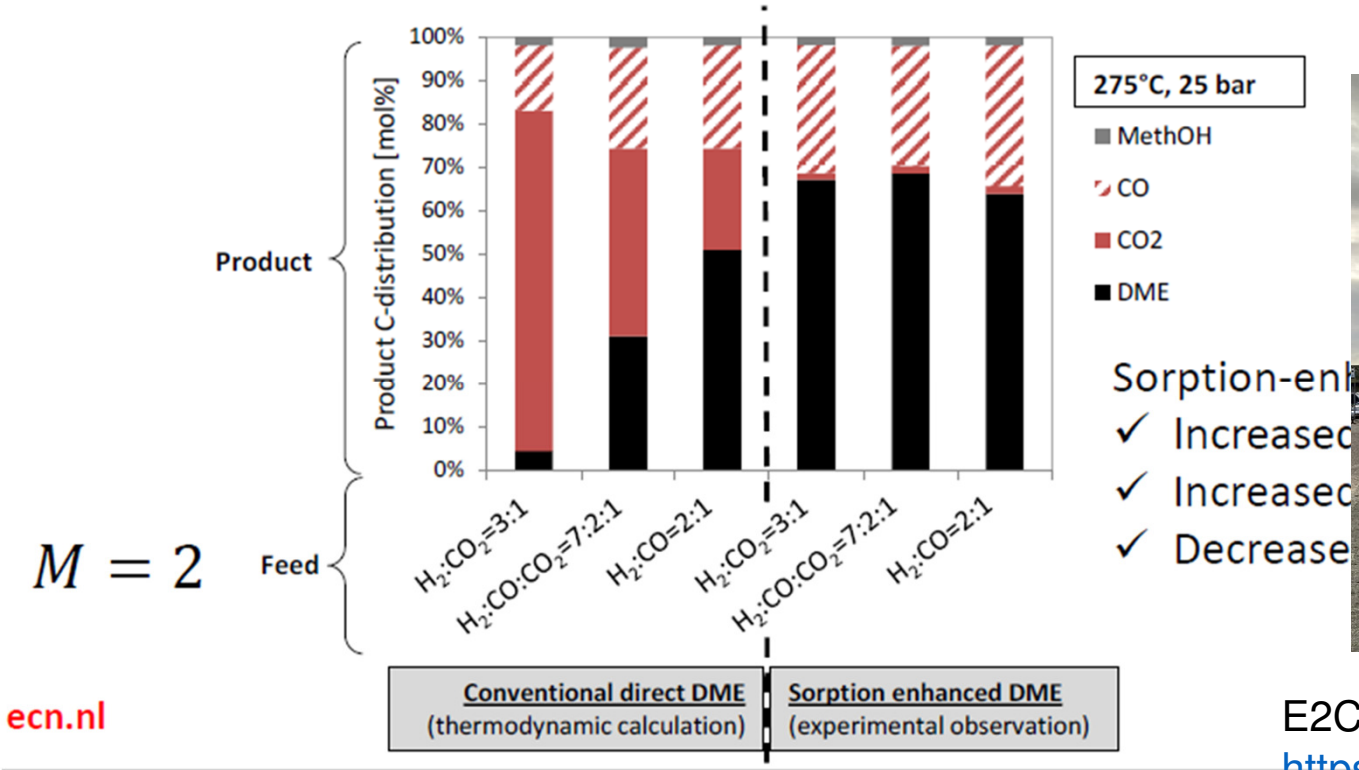
SEDMES TEST, PRESSURE SWING



Molecular sieve (adsorbent) effects:

- Extremely high DME selectivity > 90% which slowly decreases to the thermodynamic value

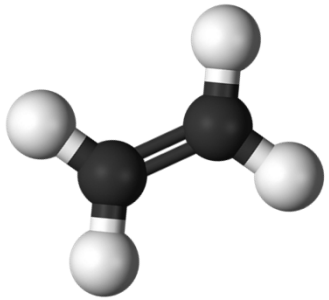
SORPTION ENHANCED DME SYNTHESIS (SEDMES)

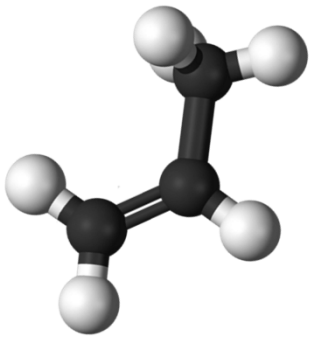


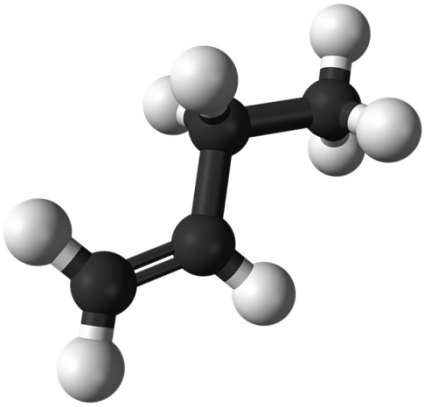
ecn.nl

E2C-Electons to Chemicals
https://www.voltachem.com/e2c

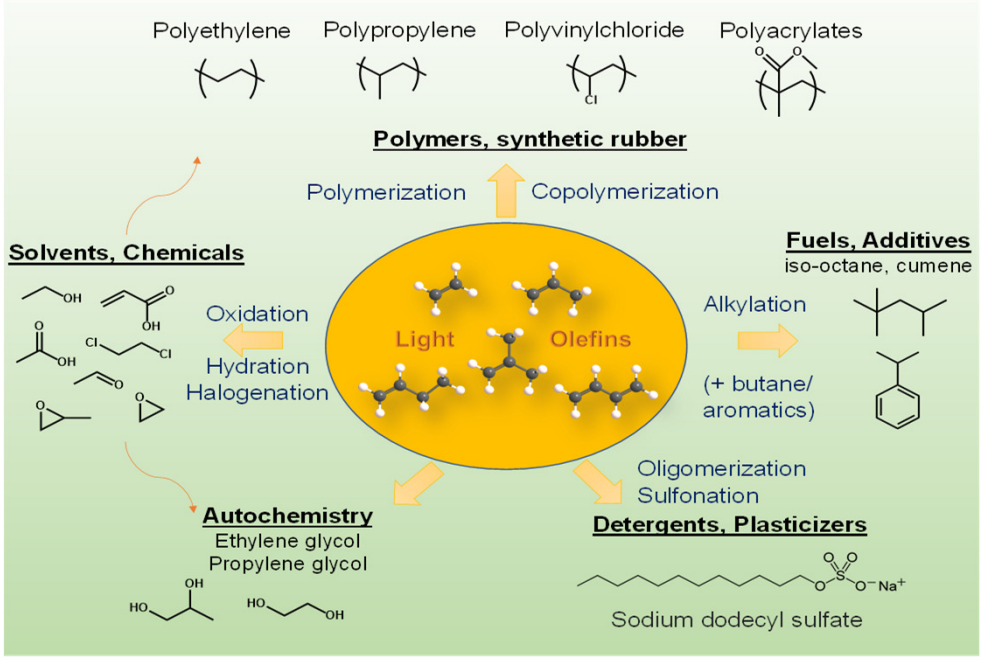
LIGHT OLEFINS

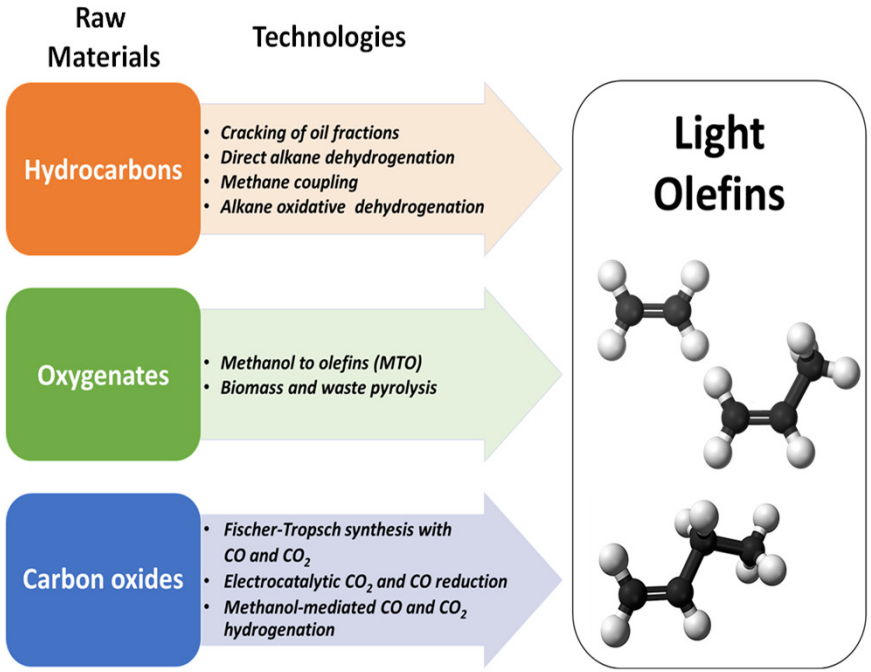






LIGHT OLEFINS, PLATFORM MOLECULES





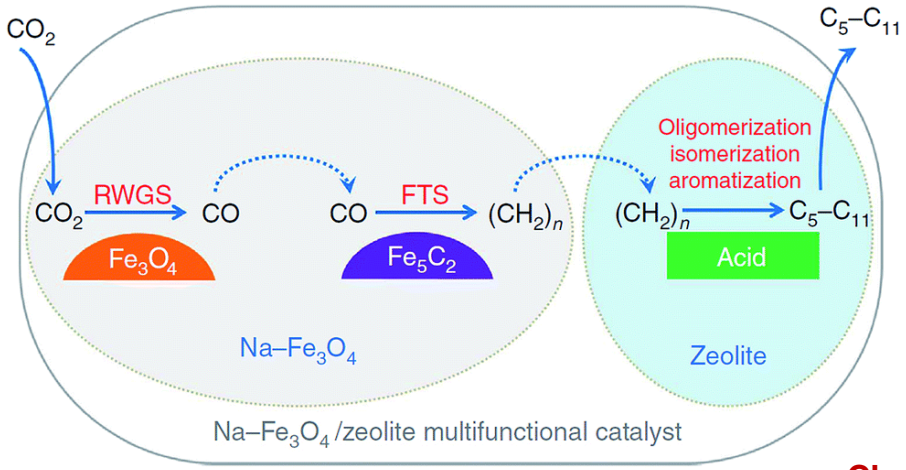
Chernyak et al, Chem. Soc. Rev. 2022

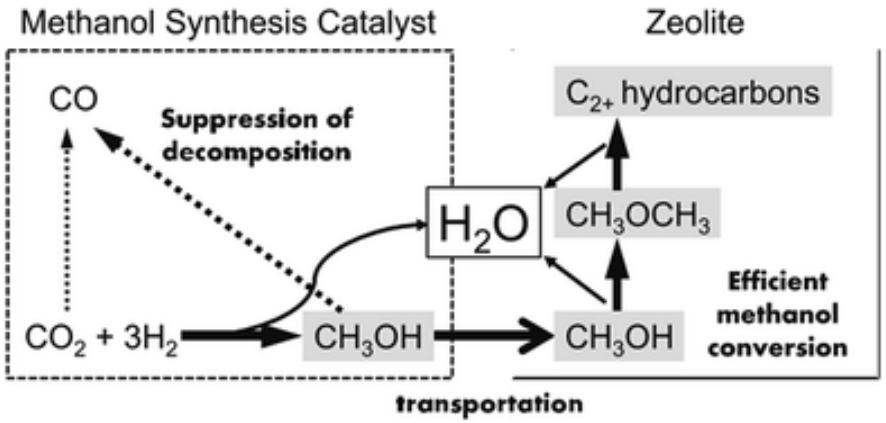
TRANSFORMING CO_2: TWO ROUTES FOR LIGHT OLEFINS SYNTHESIS

Modified Fisher-Tropsch route

Methanol-mediated synthesis route

Reverse water-gas shift reaction: $H_2+CO_2=H_2O+CO$ (favored at high temperatures)





Challenges:

Selectivity control towards specific hydrocarbons

Coproduction of CO by RWGS

Catalyst stability

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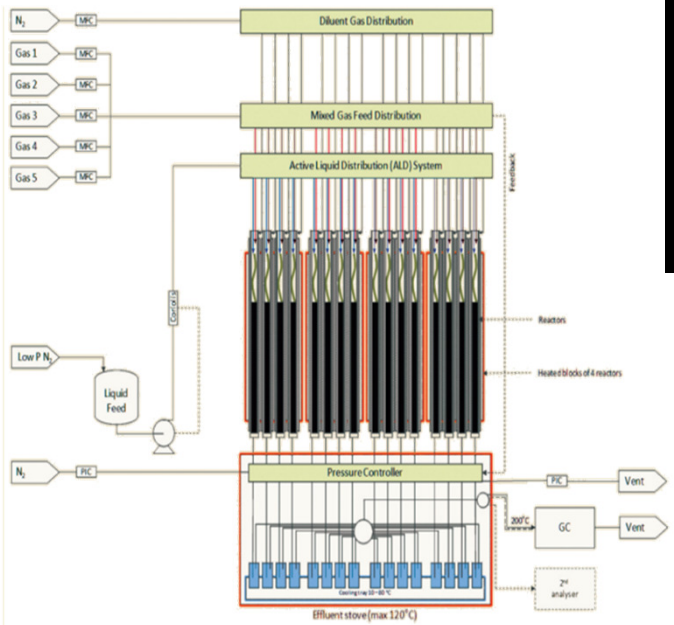
METHODOLOGY: HIGH THROUGHPUT TESTS

✓**Powerful tool for the design of new efficient heterogeneous catalysts**

✓**Different reactions such as Fischer Tropsch, VOC abatement, reforming, deNOx, oxidation, dehydration**

✓**Possibility to test 16 catalysts at the same time, using the same conditions of pressure, temperature and gas flow.**

✓**Identification of efficient promoters and selectivity trends in CO_2 hydrogenation**



Avantium Flowrence Unit, RealCat platform, Centrale Lille

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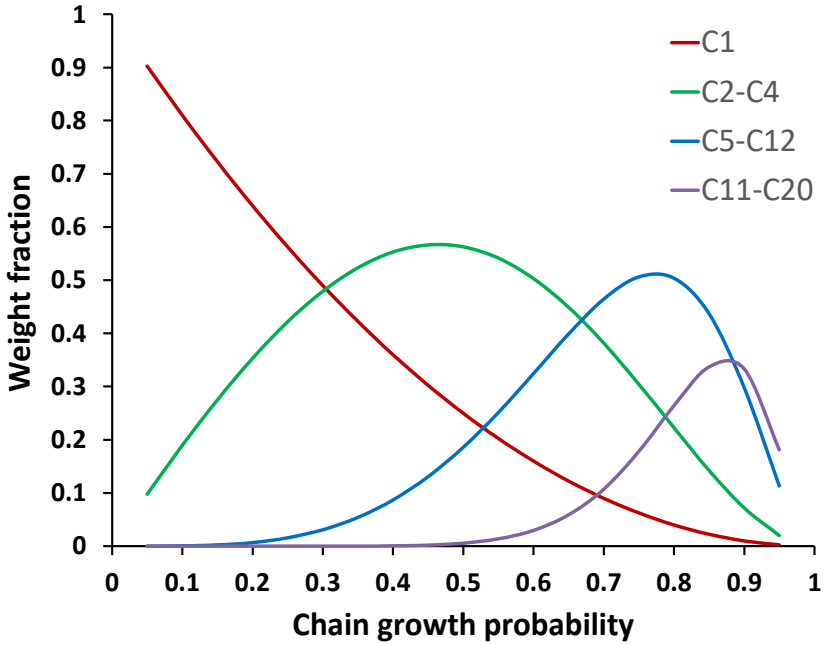
FISCHER-TROPSCH SYNTHESIS, KINETIC LIMITATIONS: ANDERSON-SCHULZ-FLORY DISTRIBUTION (α)



REVERSE WATER GAS SHIFT:

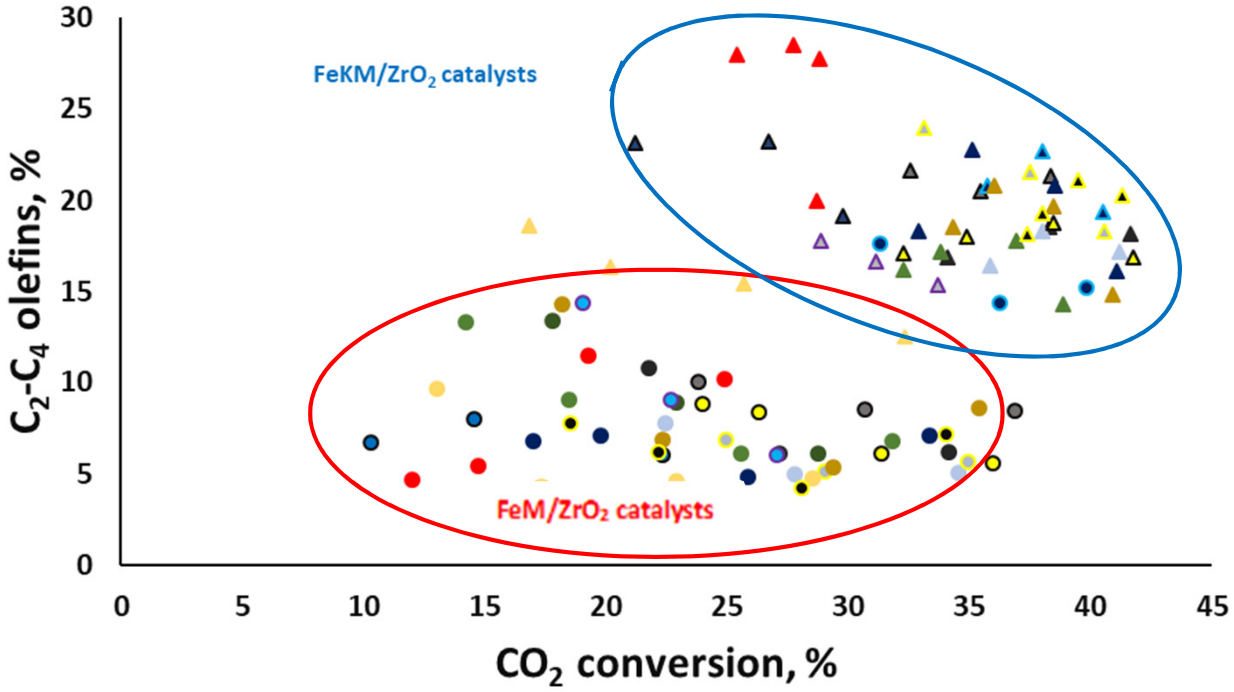
$CO_2 + H_2 \leftrightarrow CO + H_2O$ $\Delta H_R = +38$ KJ/mol

FISCHER-TROPSCH SYNTHESIS

$nCO + 2nH_2 \rightarrow C_nH_{2n} + nH_2O$ $\Delta H_R = -165$ KJ/mol

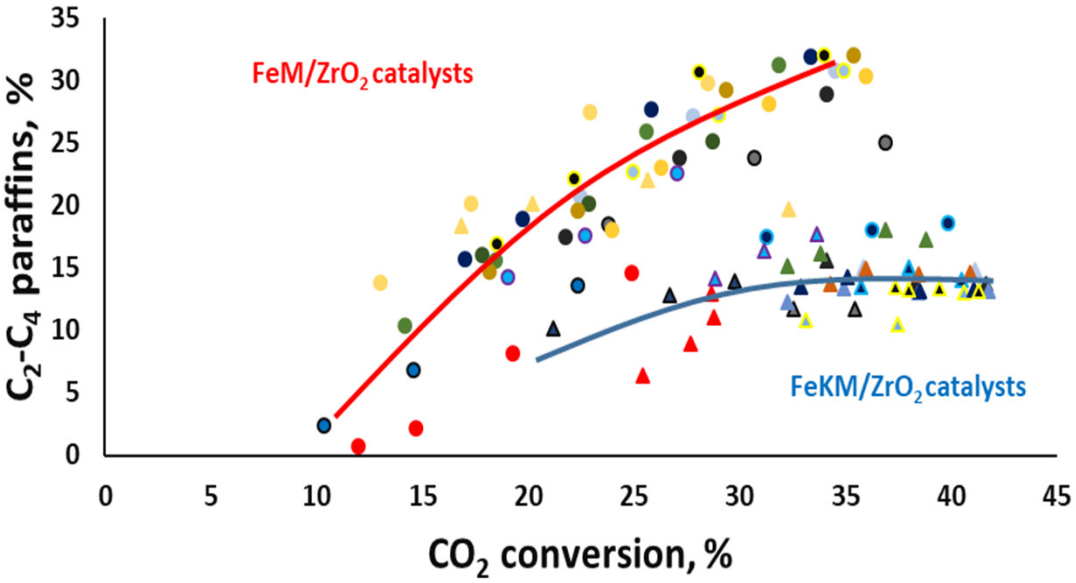
Maximum C_2-C_4 hydrocarbon selectivity is about 60%

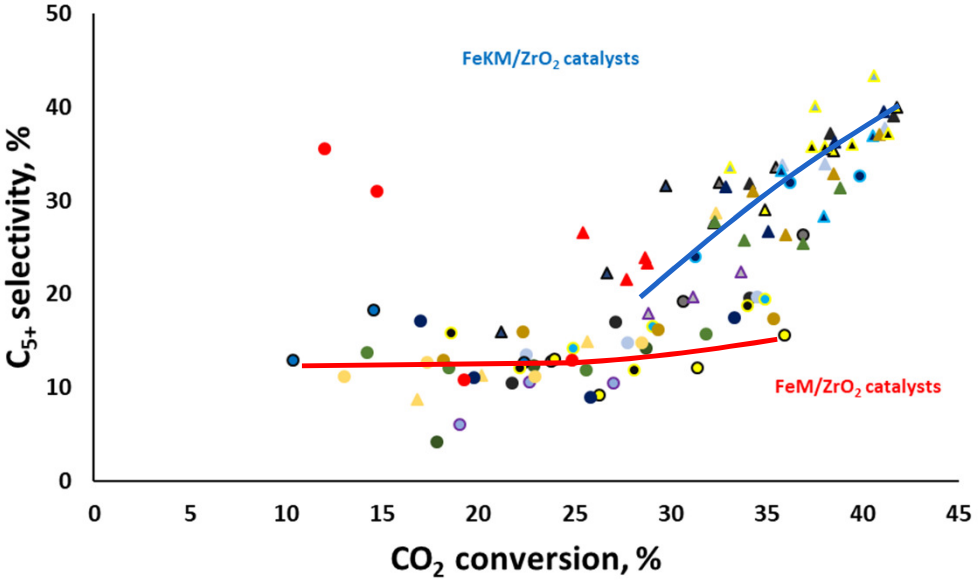
FISCHER-TROPSCH SYNTHESIS: SELECTIVITY



- Catalysts promoted with K showed the highest olefin selectivities
- Most selective catalysts to lower olefins were selected to be further studied
-
- Maximum light olefin selectivity is about 30%
- Maximum light olefin selectivity from syngas (H_2/CO) is 60%

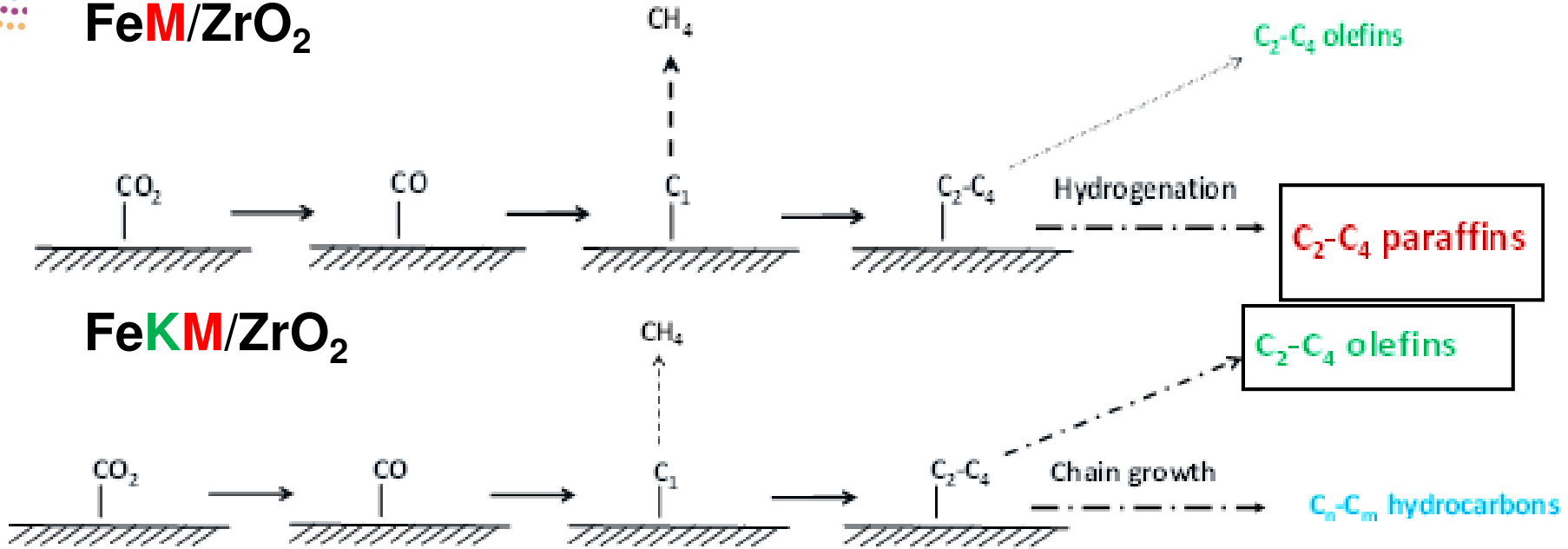
FISCHER-TROPSCH SYNTHESIS: SELECTIVITY





- ✓ **Higher paraffin selectivities are obtained with non K promoted catalysts**
- ✓ **For K promoted catalysts paraffins selectivity is rather independent of CO_2 conversion**
- ✓ **Catalysts promoted with K show the higher selectivities to C_5^+ fraction**
- ✓ **K could reduce hydrogenation ability of the catalysts favoring C-C coupling**

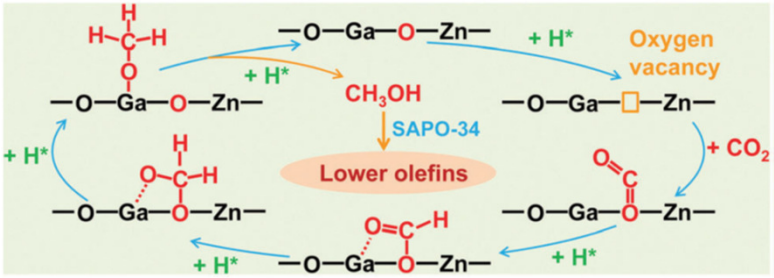
FISCHER-TROPSCH SYNTHESIS: REACTION SEQUENCE



Iron carbidization extent and basicity are crucial to improve activity and olefins selectivity
Maximum practically attained C_2-C_4 light olefin selectivity is about 30%

“Methanol Route” to Light Olefins over “Tandem” Bifunctional Catalysts

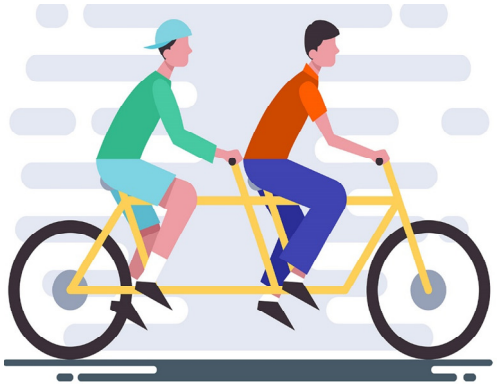
CO_2 to methanol catalysts:
Oxide component



Chem. Commun., 2018, 54, 140

MTO:

Zeolite component



One process
One reactor

CO_2 to methanol (200-300°C) < **T** < MTO (450°C)

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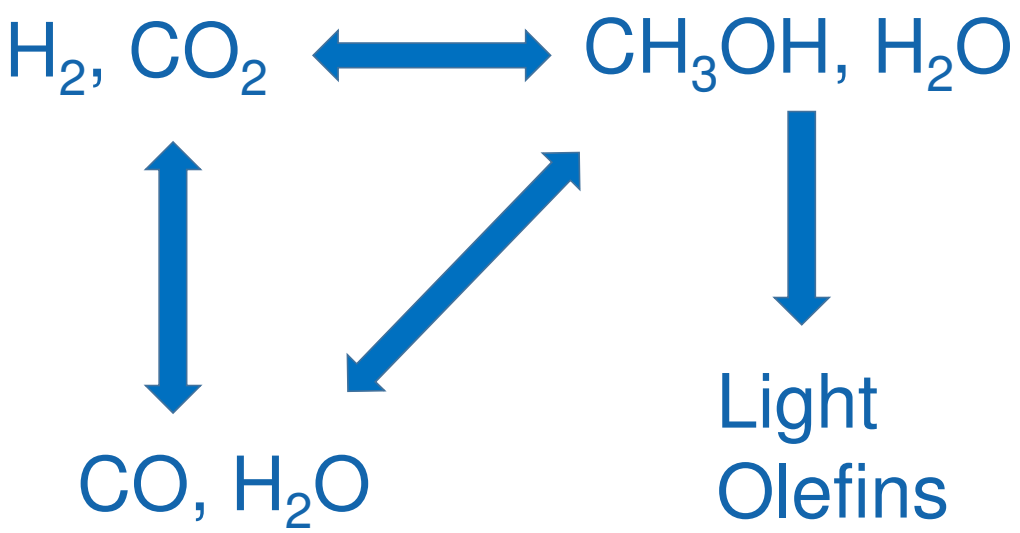
Network of Chemical Reactions and Operating Conditions



Methanol synthesis

$$CO_2 + 3\ H_2 \rightleftarrows CH_3OH + H_2O$$

$$CO + 2\ H_2 \rightleftarrows CH_3OH$$

Methanol To Olefins

$$n\ CH_3OH \rightleftarrows C_nH_{2n} + n\ H_2O$$

Reverse water gas shift

$$CO_2 + H_2 \rightleftarrows CO + H_2O$$

Secondary hydrogenation

$$C_nH_{2n} + H_2 \rightarrow C_nH_{2n+2}$$

Intermediate temperature and pressure between methanol synthesis and MTO ≈350-400°C, 20-30 bar

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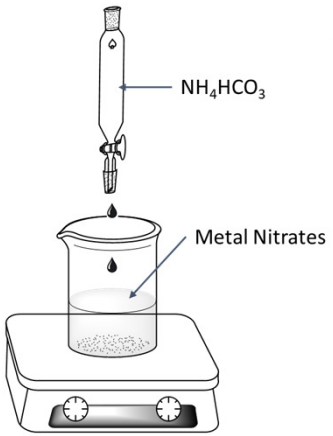
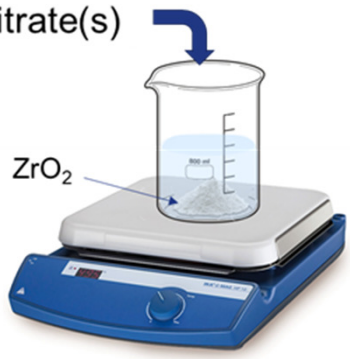
Catalyst Design: Metal-Oxide Component

Numerous metal-oxide catalysts were tested:



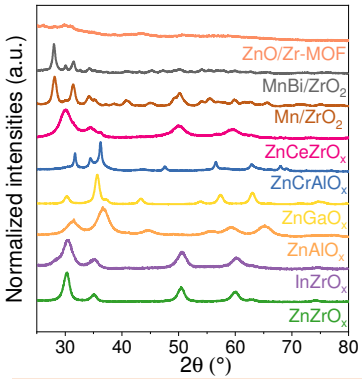
Co-precipitation



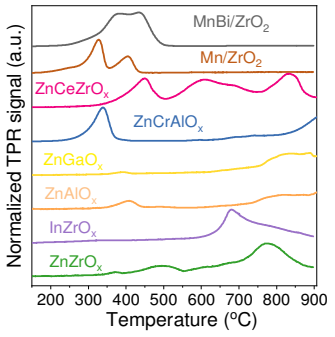
Impregnation

- Different compositions and structure
- Different reducibility
- Different types of basic sites and their relative concentration

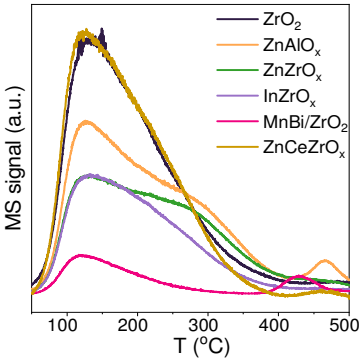
XRD



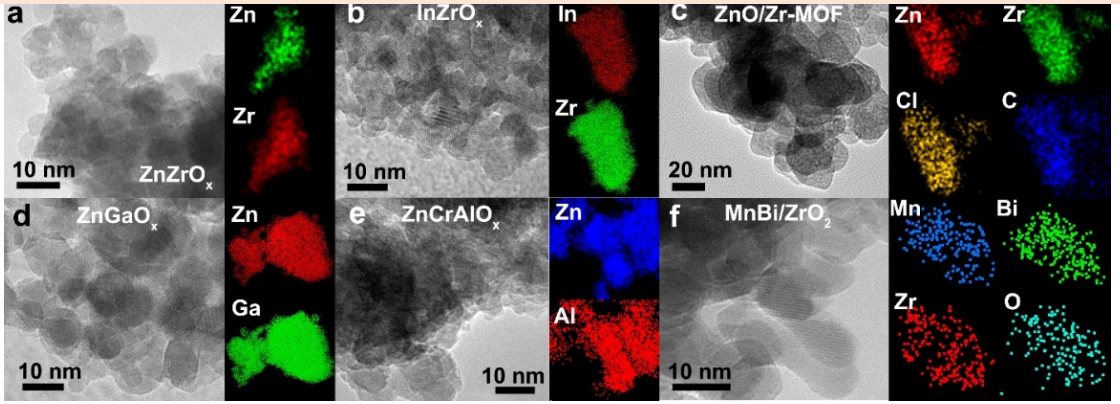
H_2-TPR



CO_2-TPD



TEM



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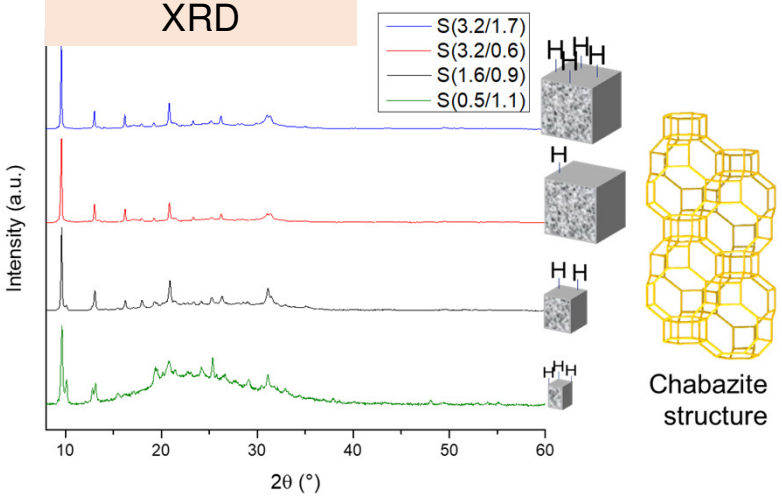
Catalyst Design: SAPO-34 Zeolite Component

XRD



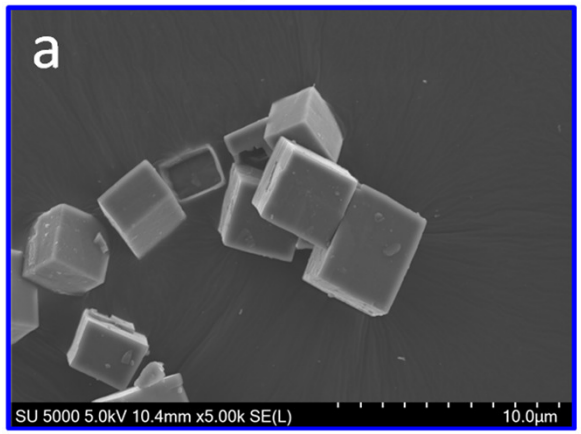
Chabazite structure

Zeolite	Crystallite size, µm	Acid density, mmol/g
S(3.2/1.7)	3.2	1.67
S(3.2/0.6)	3.2	0.61
S(1.6/0.9)	1.6	0.95
S(0.5/1.1)	0.5	1.14

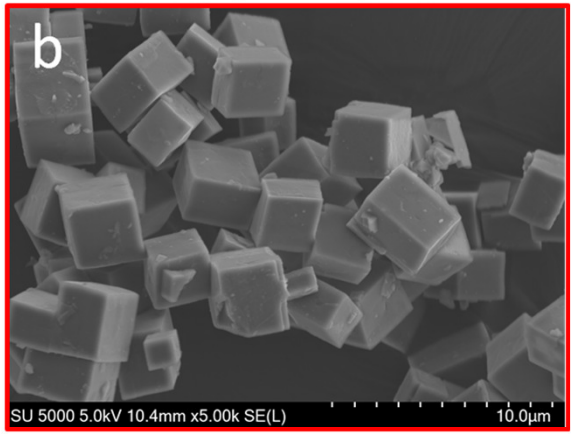
The chosen SAPO-34 samples are named
S(particle size(µm)/acid density(mmol/g))

SEM

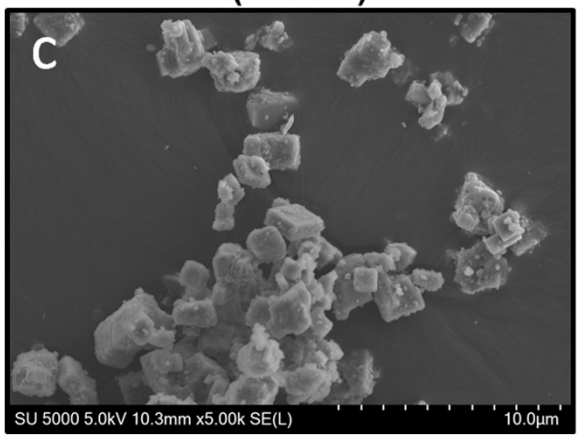
S(3.2/1.7)



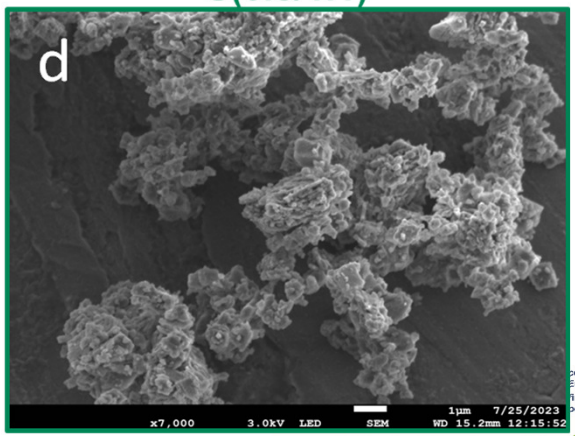
S(3.2/0.6)



S(1.6/0.9)



S(0.5/1.1)



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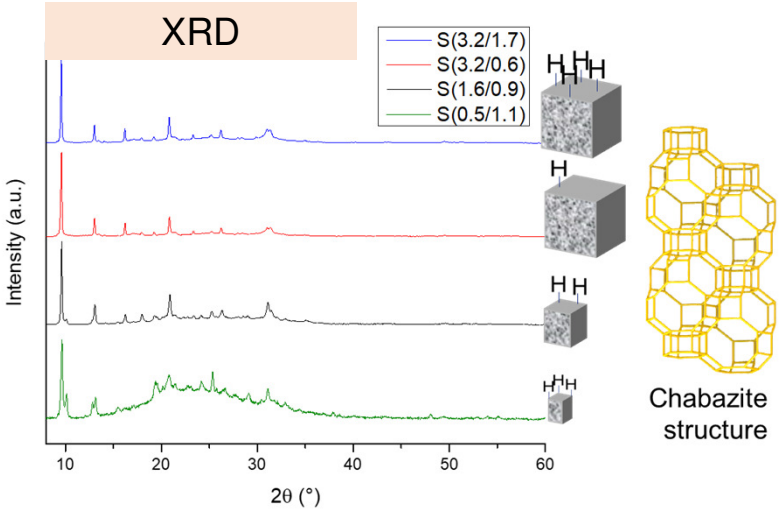
Catalyst Design: SAPO-34 Zeolite Component

XRD



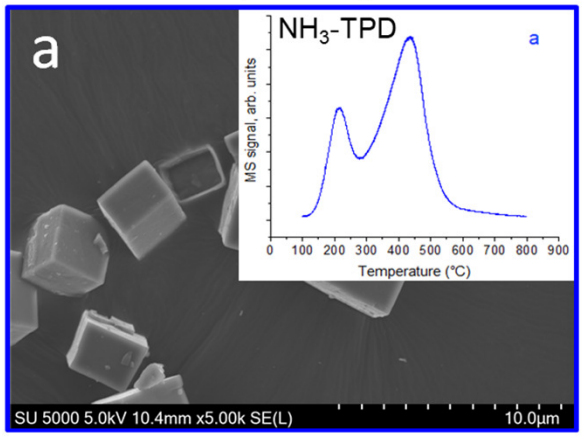
Chabazite structure

Zeolite	Crystallite size, µm	Acid density, mmol/g
S(3.2/1.7)	3.2	1.67
S(3.2/0.6)	3.2	0.61
S(1.6/0.9)	1.6	0.95
S(0.5/1.1)	0.5	1.14

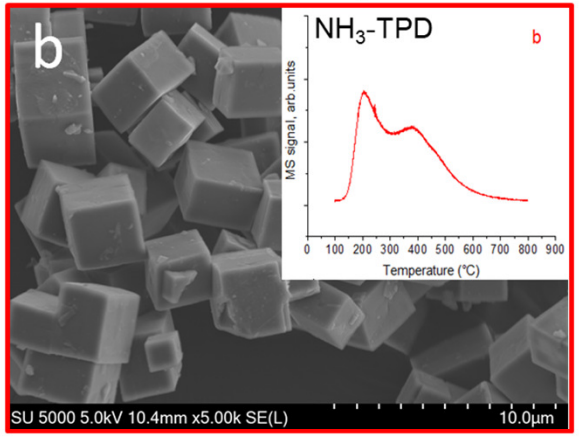
The chosen SAPO-34 samples are named S(particle size(µm)/acid density(mmol/g))

NH_3-TPD

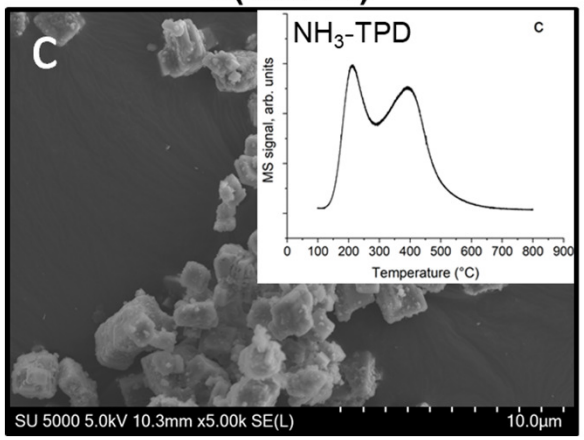
S(3.2/1.7)



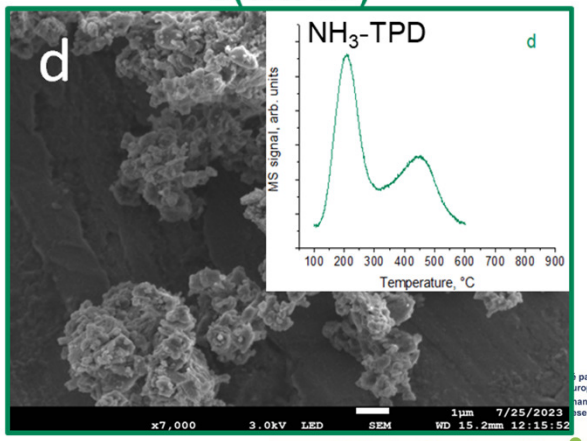
S(3.2/0.6)



S(1.6/0.9)



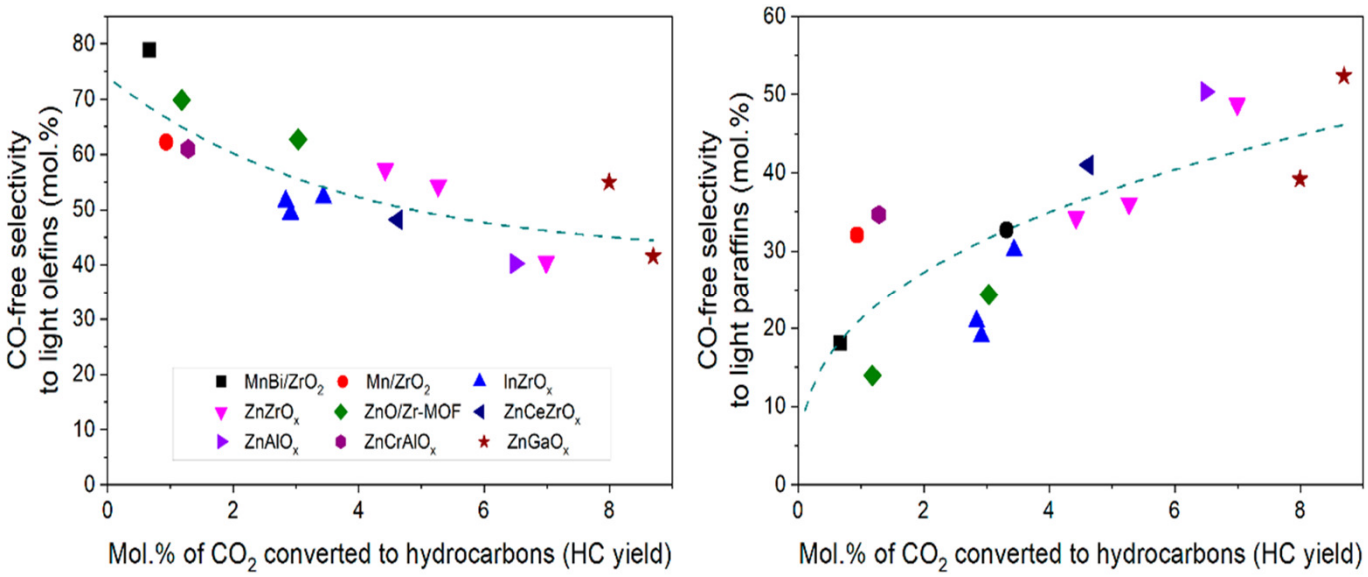
S(0.5/1.1)



CO_2 Hydrogenation to Light Olefins: Selectivity-Conversion Correlations

- High-throughput screening of bi-finctional catalysts
- No evident dependance of selectivity to LO on CO_2 conversion
- Dependence of CO-free selectivity to LO on HC yield
- The higher the CO_2 conversion to HC, the higher the possibility that LO are further hydrogenated to LP

Metal-oxides mixed with S(3.2/1.7) in 1:1 ratio



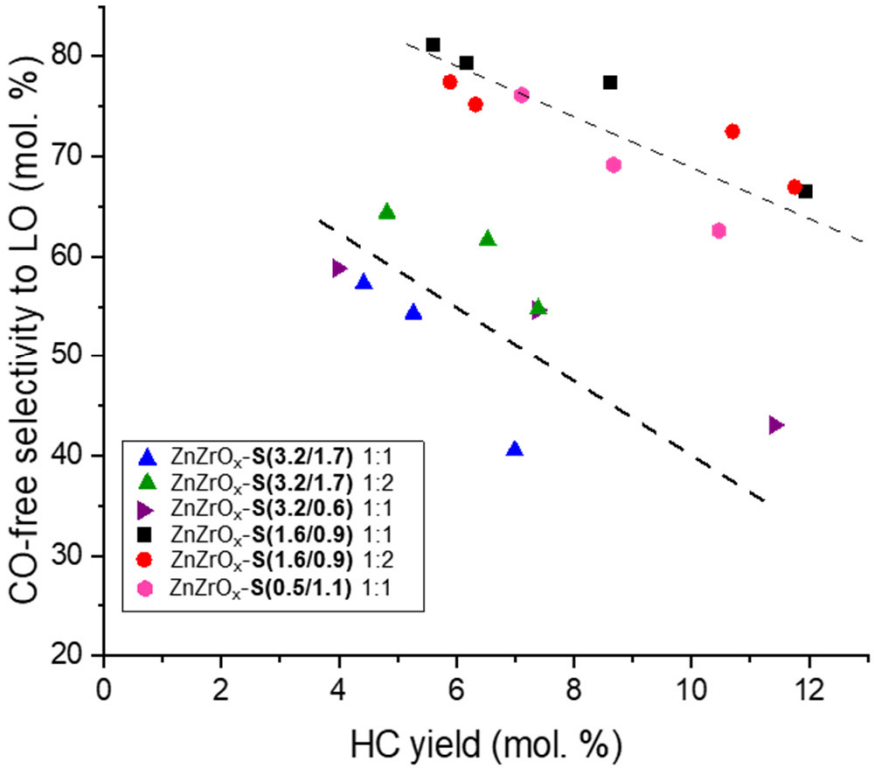
Conditions: 375°C, 20 bar, WHSV of 1000-3000 NL/g_{cat}/h.

Zeolite Influence on Selectivity to Light Olefins: Different zeolites

Zeolite	Particle size, µm	Acid density, mmol/g
S(3.2/1.7)	3.2	1.67
S(3.2/0.6)	3.2	0.61
S(1.6/0.9)	1.6	0.95
S(0.5/1.1)	0.5	1.14

$ZnZrO_x$ mixed with different SAPO-34 zeolites

The chosen SAPO-34 samples are named
S(particle size(µm)**/**acid density(mmol/g)**)**



Conditions: WHSV of 1-3 NL g_{cat}^{-1} h^{-1}, 20 bar, and 375 °C

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Zeolite Influence on Selectivity to Light Olefins
Different Zeolites

Zeolite	Particle size, µm	Acid density, mmol/g
S(3.2/1.7)	**3.2**	1.67
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S(1.6/0.9)	**1.6**	0.95
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- Smaller zeolite crystallites improve the selectivity to LO

The chosen SAPO-34 samples are named
S(particle size(µm)/acid density(mmol/g))

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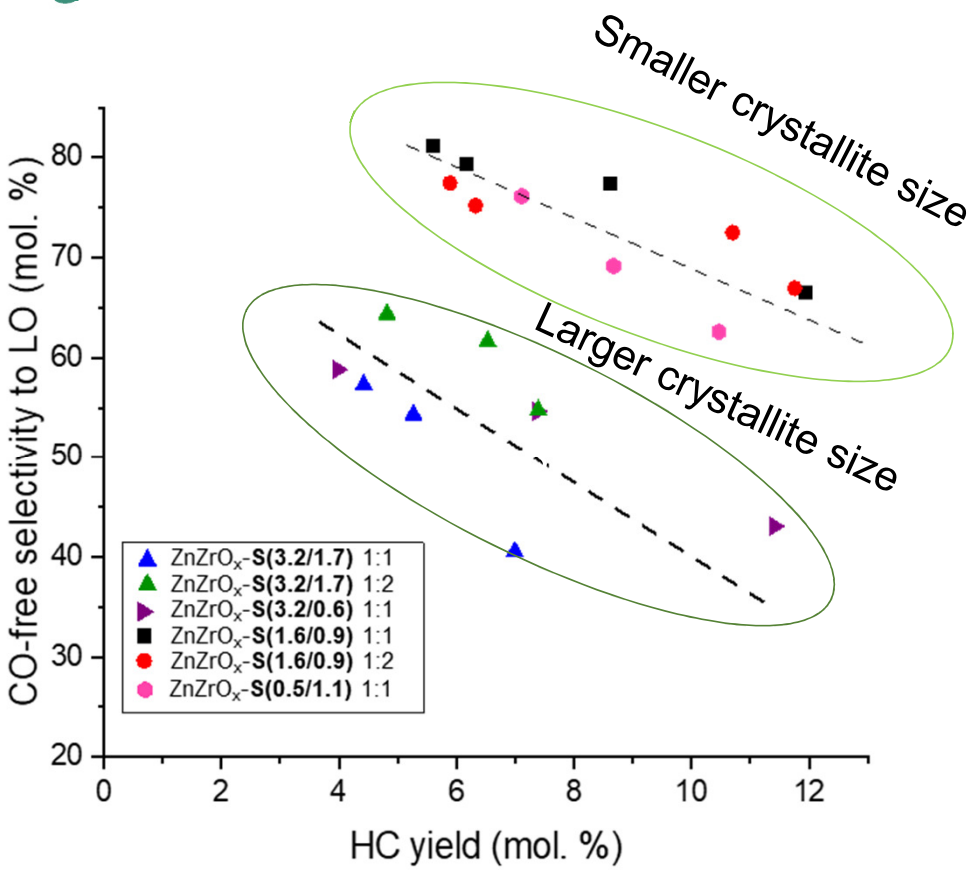

Conditions: WHSV of 1-3 NL g_{cat}^{-1} h^{-1}, 20 bar, and 375 °C

Zeolite Influence on Selectivity to Light Olefins
Different Zeolites

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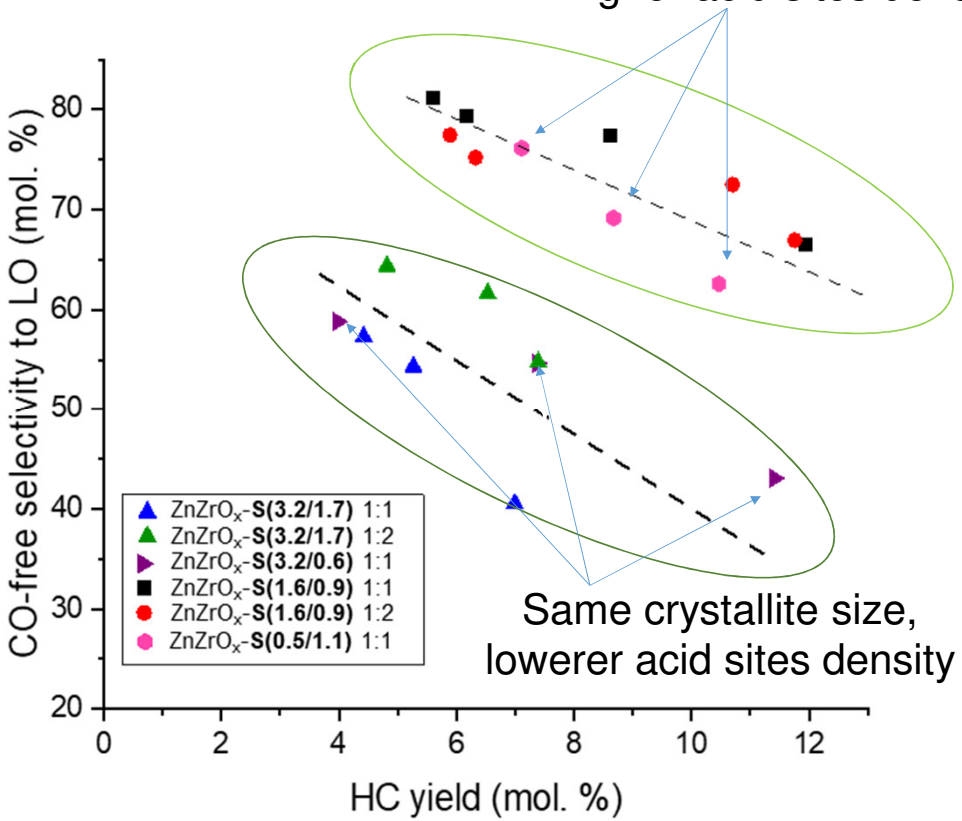
S(3.2/0.6)	**3.2**	**0.61**
S(1.6/0.9)	**1.6**	0.95
S(0.5/1.1)	**0.5**	**1.14**

- To a minor extent, less acidic zeolites increase selectivity to LO

The chosen SAPO-34 samples are named
S(particle size(µm)/acid density(mmol/g)**)**

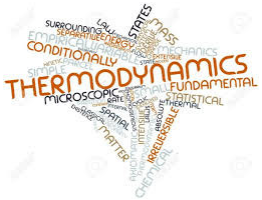
Smaller crystallite size, higher acid sites density



Same crystallite size, lowerer acid sites density

Conditions: WHSV of 1-3 NL g_{cat}^{-1} h^{-1}, 20 bar, and 375 °C

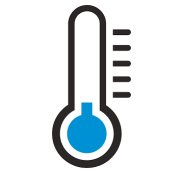
CONCLUSION
CHALLENGES AND SOLUTIONS FOR CO_2 HYDROGENATION

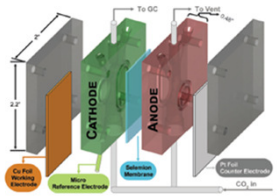


CHALLENGES

- Availability of cheap and “green” hydrogen
- Selectivity can be insufficient for industrial application, co-production of CO
- Unfavorable thermodynamics of most of CO_2 related reactions
- Competitive cost of the CO_2-based fuels and chemicals relative to the existing market solutions.

SOLUTIONS





- Development of new technologies for the production of sustainable hydrogen
- Development of catalysts operating at lower temperatures, lower energy consumption, increase in the product selectivity
- Chemical and engineering strategies to improve the thermodynamics (addition of different compounds (usually amines, alkali or ethers) to the feed, transient operation, chemical looping, SEDMES)
- Elaboration of electrocatalytic processes for direct CO_2 reduction

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