Catalyst Design for Efficient Hydrogen Production & Storage in Chemical Hydrogen Carriers

Prof. Dr. Regina Palkovits

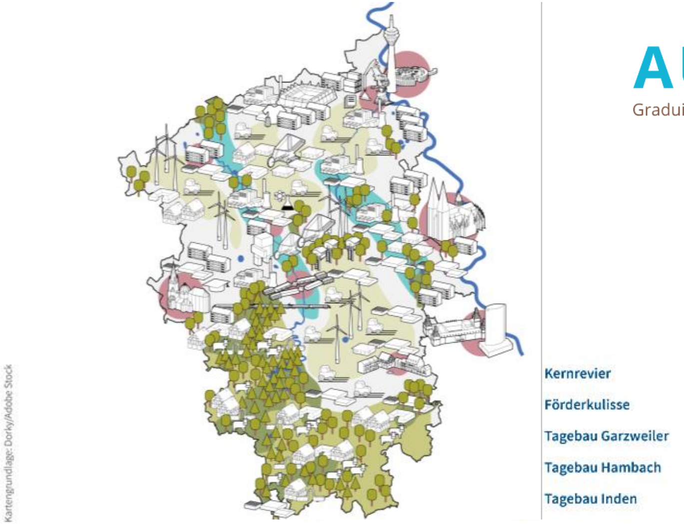
r.palkovits@fz-juelich.de
palkovits@itmc.rwth-aachen.de

@PalkovitsLab

JÜLICH Forschungszentrum | RWTH AACHEN UNIVERSITY

Hydrogen & Bioeconomy Transformation of Rhine District

STRUKTURWANDEL
RHEINISCHES
REVIER



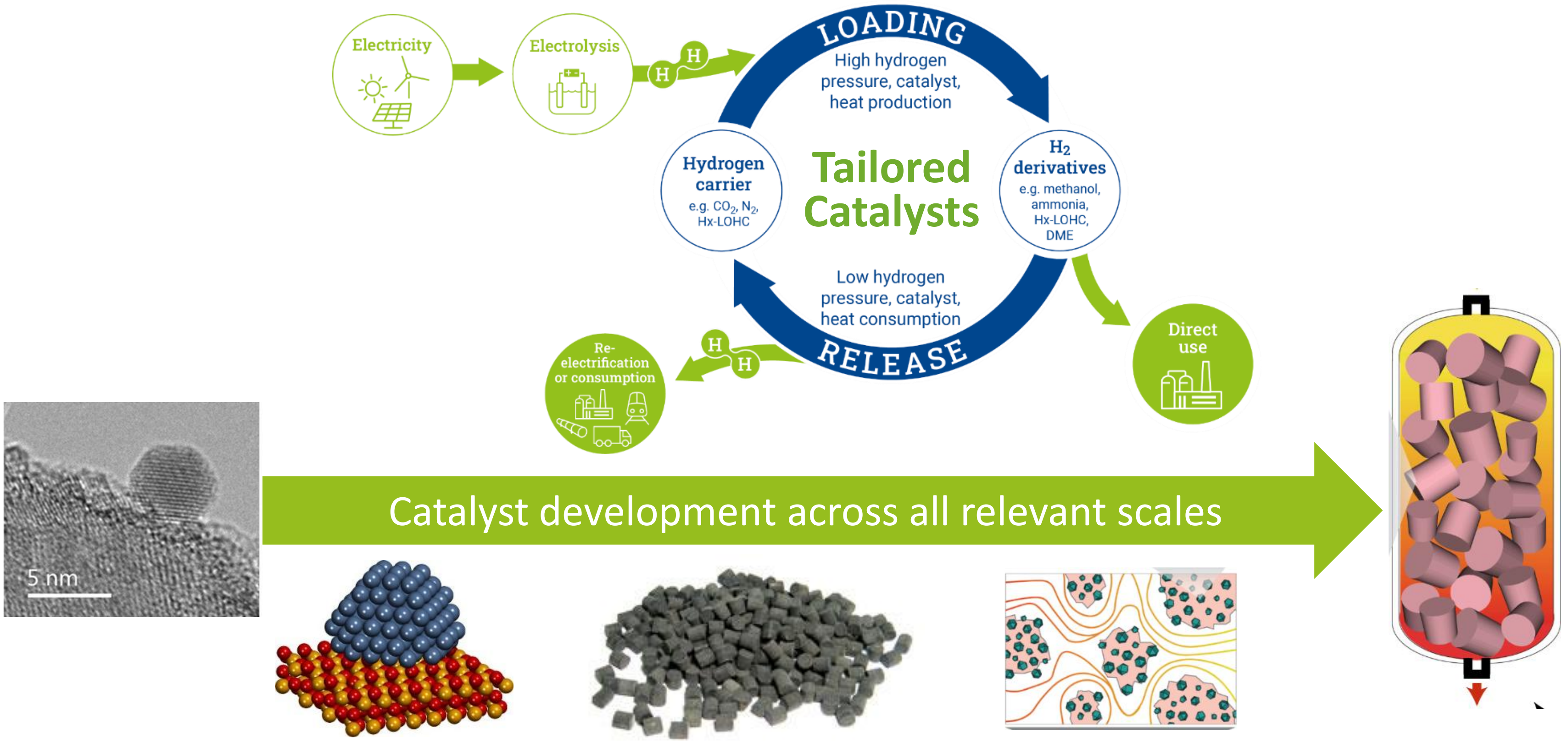
AUFBRUCH
Graduiertencluster Nachhaltiges Revier

Innovation Valley

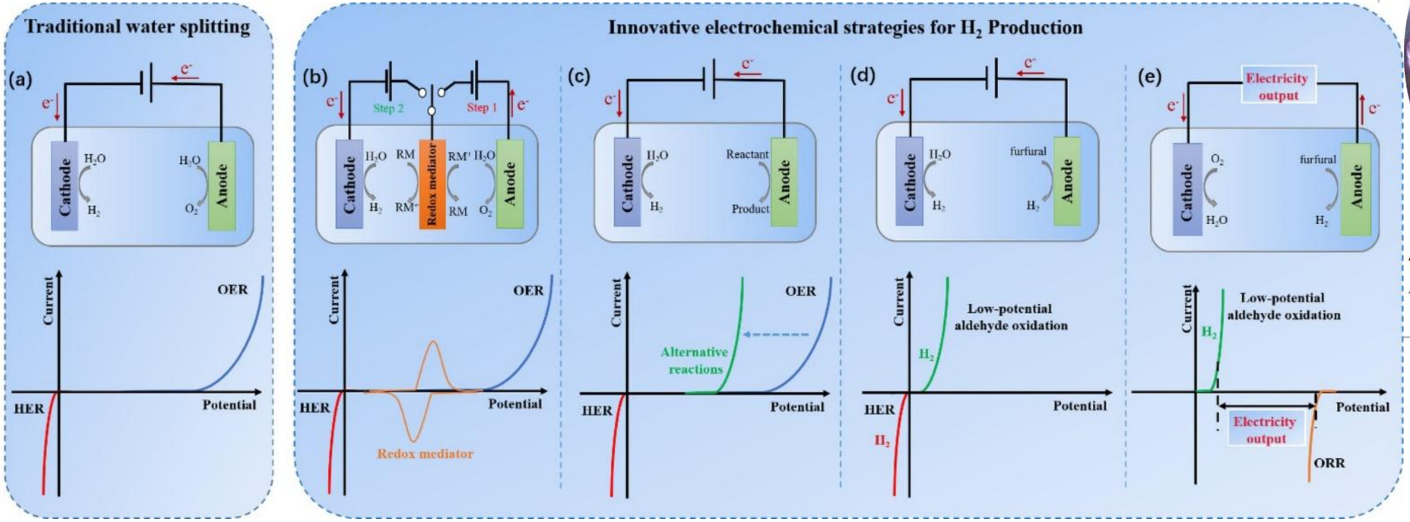
HC·H2
Helmholtz-Cluster
Wasserstoff

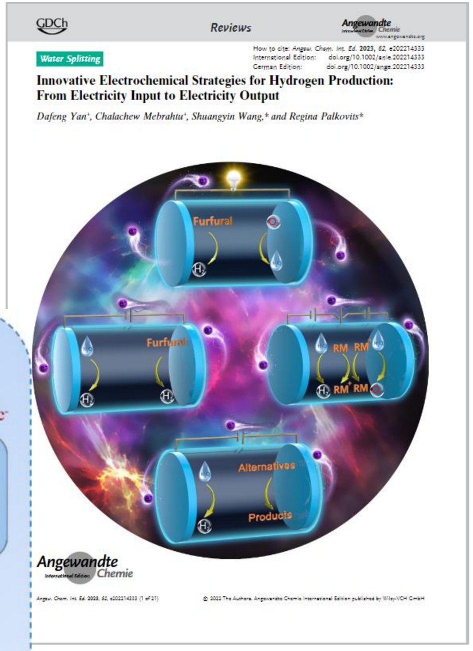
Chemical hydrogen carriers

Enabling long-term storage and long-distance transportation



Efficient electrocatalytic transformations




GDCh Reviews Angewandte Chemie

Water Splitting

How to cite: Angew. Chem. Int. Ed. 2023, 62, e202214333
International Edition: doi.org/10.1002/anie.202214333
German Edition: doi.org/10.1002/ange.202214333

Innovative Electrochemical Strategies for Hydrogen Production: From Electricity Input to Electricity Output

Dafeng Yan+, Chalachew Mebrahtu+, Shuangyin Wang, and Regina Palkovits**

Angewandte Chemie

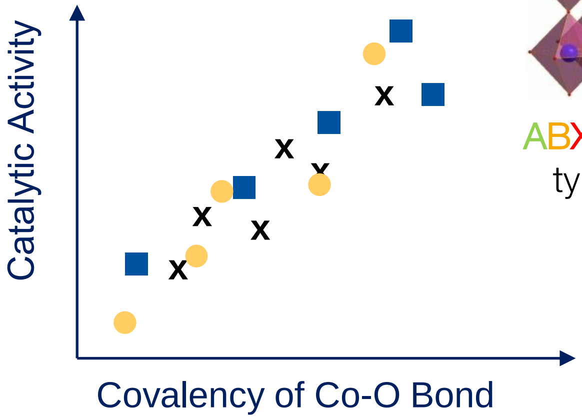
Angew. Chem. Int. Ed. 2023, 62, e202214333 (1 of 21)

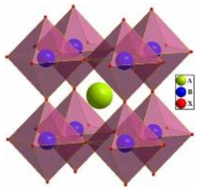
© 2022 The Authors. Angewandte Chemie International Edition published by Wiley-VCH GmbH

D. Yan, C. Mebrahtu, S. Wang, R. Palkovits, *Angew. Chem. Int. Ed.* **2023**, 62, e202214333

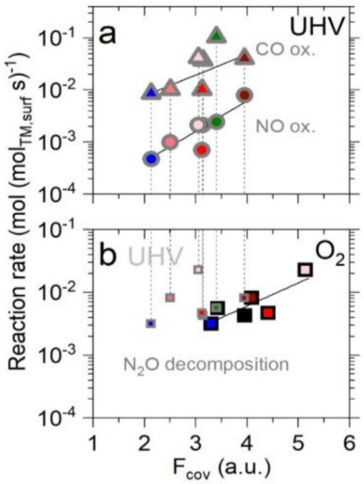
JÜLICH Forschungszentrum RWTH AACHEN UNIVERSITY

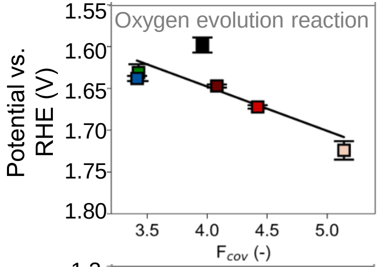
Descriptor-based Catalyst Design

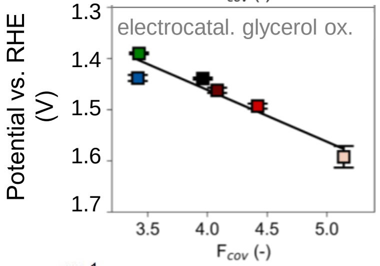


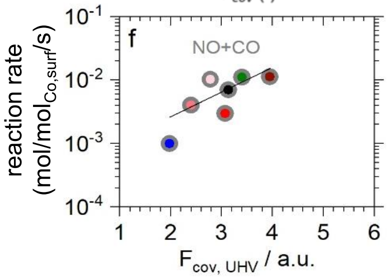


ABX_3: perovskite-type structure









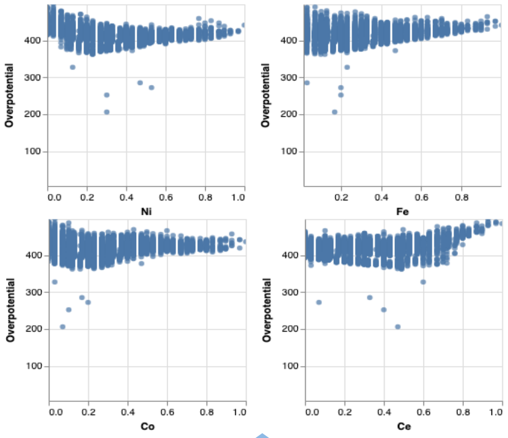
Catalyst description by bulk property across chemo- and electrocatalysis!

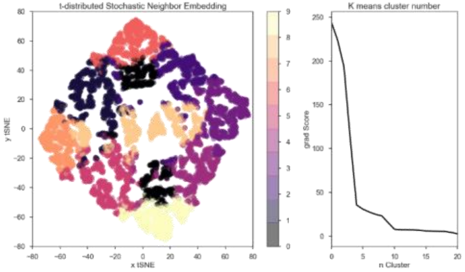
J. Simböck, M. Ghiashi, S. Schönebaum, U. Simon, F.M.F. de Groot, R. Palkovits, *Nat. Commun.* **2020**, 11, 652

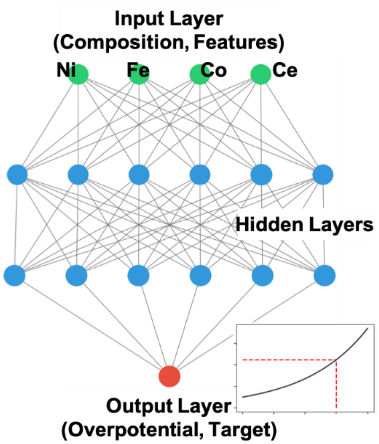
S. Mürtz, J. Simböck, F. Zeng, M. Ghiasi, S. Schönebaum, U. Simon, F. M.F. de Groot, R. Palkovits, *EES Catal.* **2023**, D3EY00206C

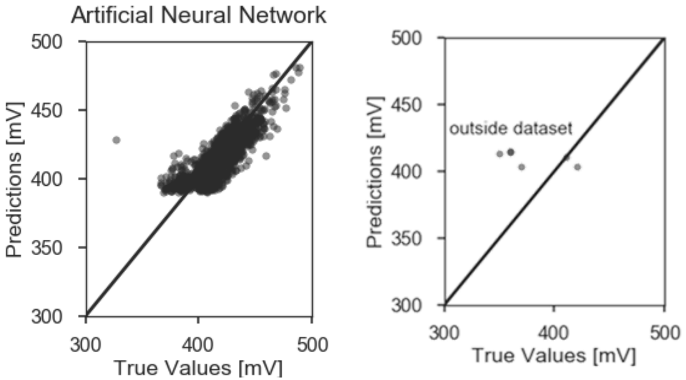
JÜLICH Forschungszentrum RWTHAACHEN UNIVERSITY

Data Science-based Description of OER catalysts



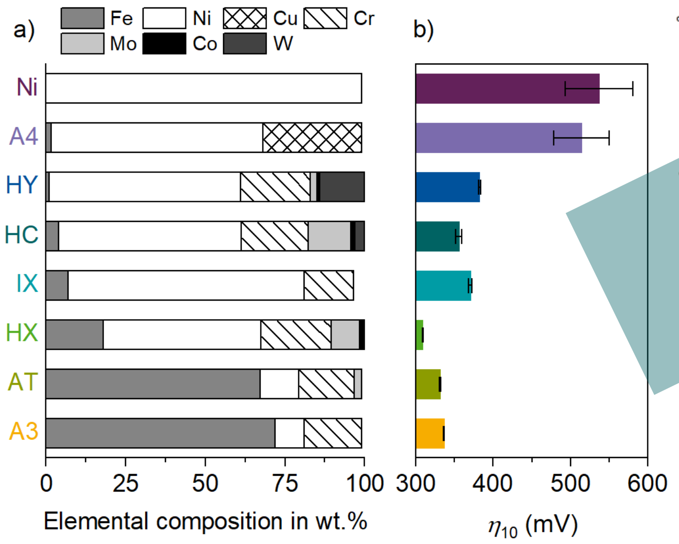


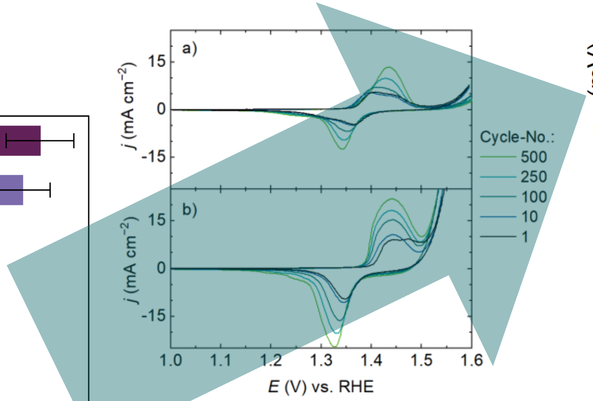


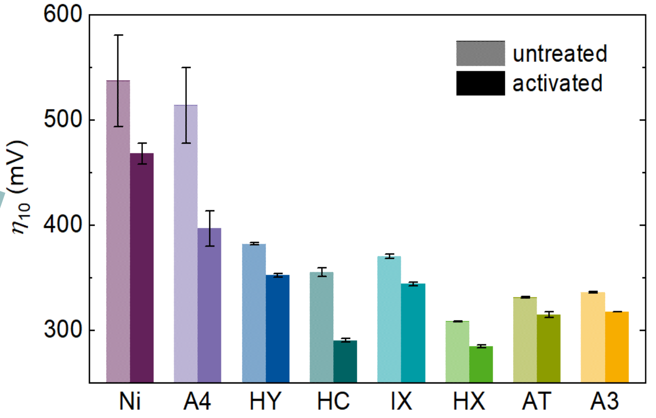


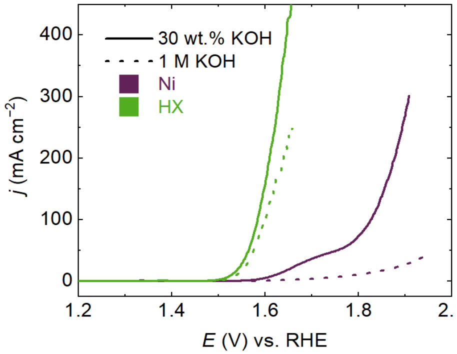
R. Palkovits, S. Palkovits, *ACS Catal.* **2019**, 9, 9, 8383–8387
S. Palkovits, *ChemCatChem* **2020** 12, 3995-4008

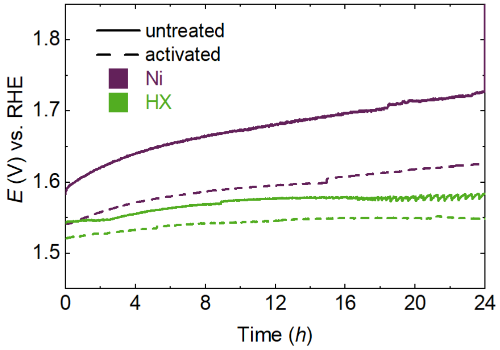
Activation of Commercial Ni Alloys







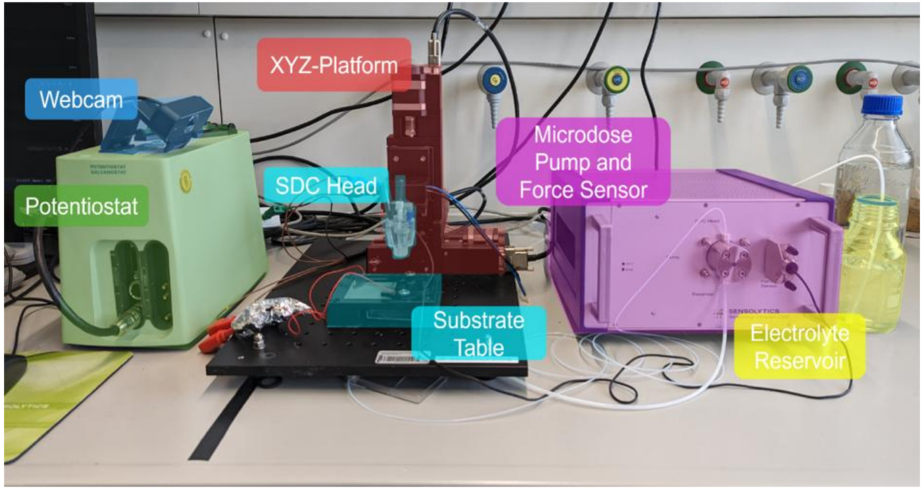


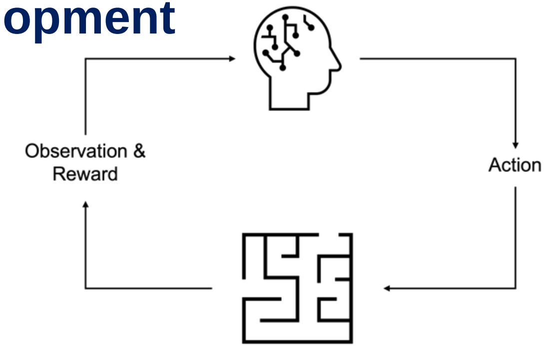


M. Kubo, F. Ketter, S. Palkovits, R. Palkovits*, *ChemElectroChem.* **2024** 11 (6), e202300460,
https://doi.org/10.1002/celc.202300460
Zenodo **2024**, doi. 10.5281/zenodo.10669810

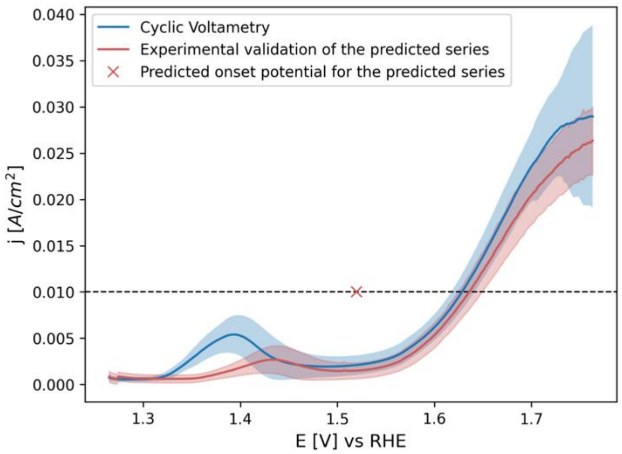
Self-optimizing Automated Electrocatalyst Development

Automated Lab Equipment: Scanning droplet cell for high-throughput experimentation





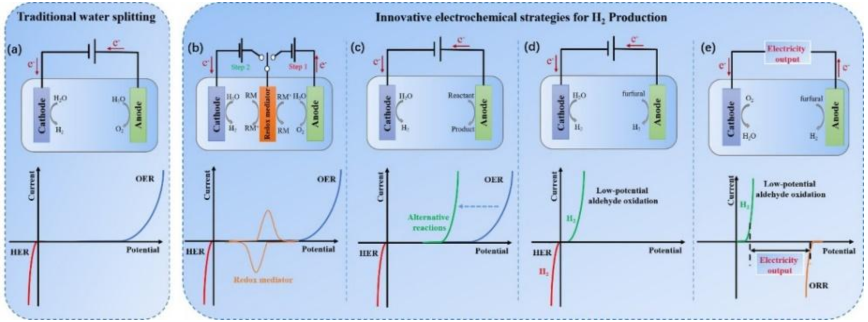
Experiment design with ML

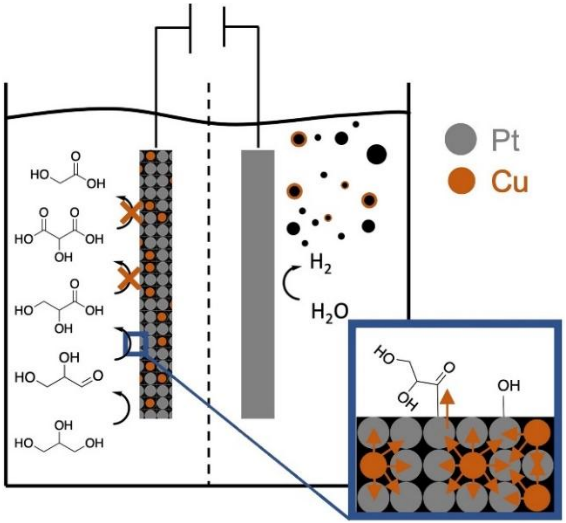


H. Spitzenpfeil, M. Neumann, N. Hausen, R. Palkovits, S. Palkovits, **2025** submitted

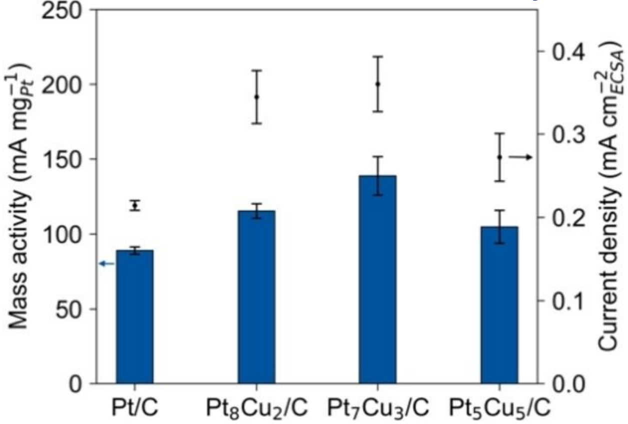
JÜLICH Forschungszentrum RWTHAACHEN UNIVERSITY

Efficient electrocatalytic transformations

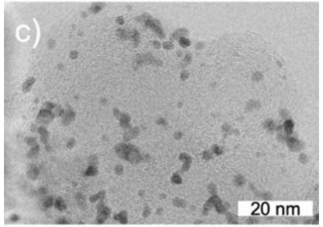




Normalized Pt mass activity



1.1 V vs. RHE for GOR vs. acidic OER on IrO_2 at 1.52 V

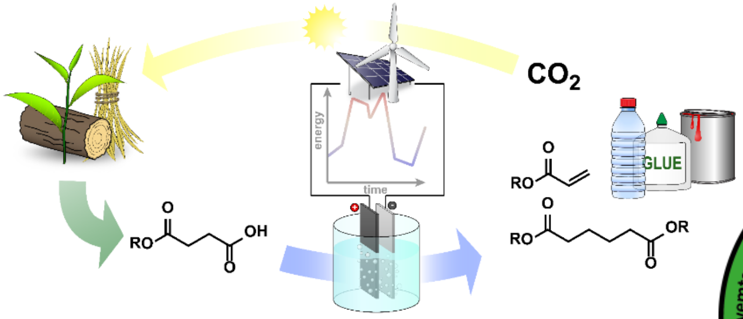


0.5 M H_2SO_4 with 2 M glycerol, 20 mV s^{-1} scan rate.

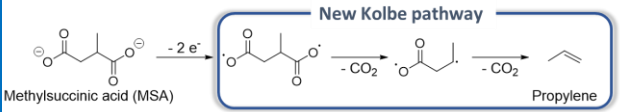
S. D. Mürtz, F. Musialek, N. Pfänder, R. Palkovits, *ChemElectroChem.* **2023**, e202201114
Dataset: Zenodo doi.10.5281/zenodo.8113211
D. Yan, C. Mebrahtu, S. Wang, R. Palkovits, *Angew. Chem. Int. Ed.* **2023**, 62, e202214333

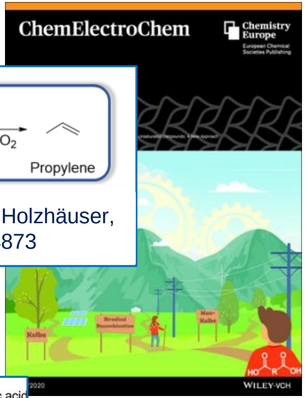
JÜLICH Forschungszentrum RWTHAACHEN UNIVERSITY

Kolbe/non-Kolbe Electrolysis @ PalkovitsLab

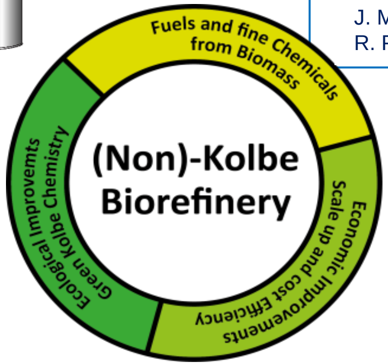


G. Creusen, F. J. Holzhäuser, J. Artz, S. Palkovits, R. Palkovits, *ACS Sust. Chem. Eng.* **2018**, 6, 17108



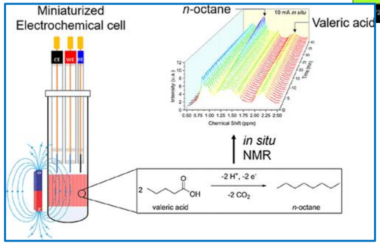


J. Meyers, N. Kurig, M. Valeske, S. Panitz, F. J. Holzhäuser, R. Palkovits, *ChemElectroChem.* **2020**, 7 (24), 4873

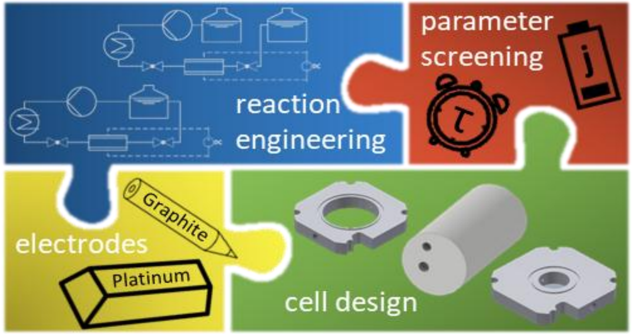


F. J. Holzhäuser, J. B. Mensah, R. Palkovits, *Green Chem.* **2020**, 22, 286

S. Palkovits, R. Palkovits, *Chem. Ing. Technik*, **2019**, 91, 6, 699

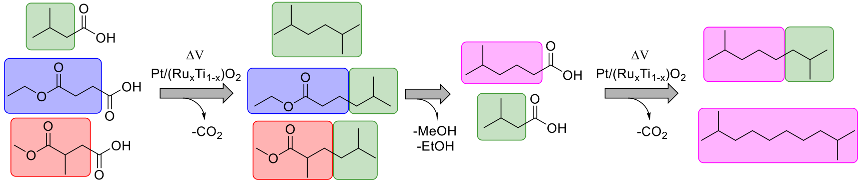


J. Holzhäuser, G. Creusen, G. Moos, M. Dahmen, A. König, J. Artz, S. Palkovits, R. Palkovits, *Green Chem.* **2019**, 21, 2334



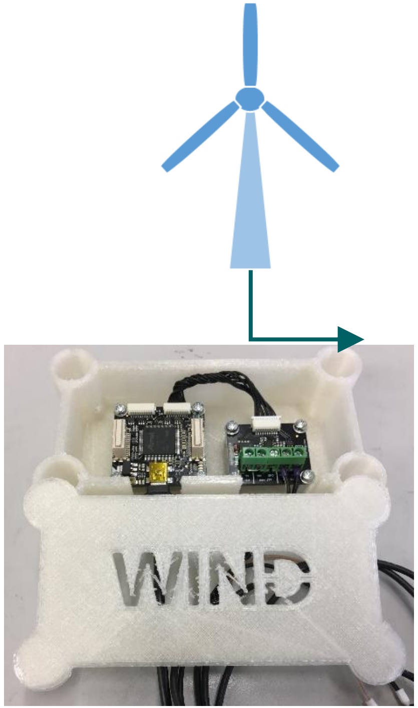
N. Kurig, J. Meyers, F. J. Holzhäuser, S. Palkovits, R. Palkovits, *ACS Sustain. Chem. Eng.* **2021**, 9, 3, 1229

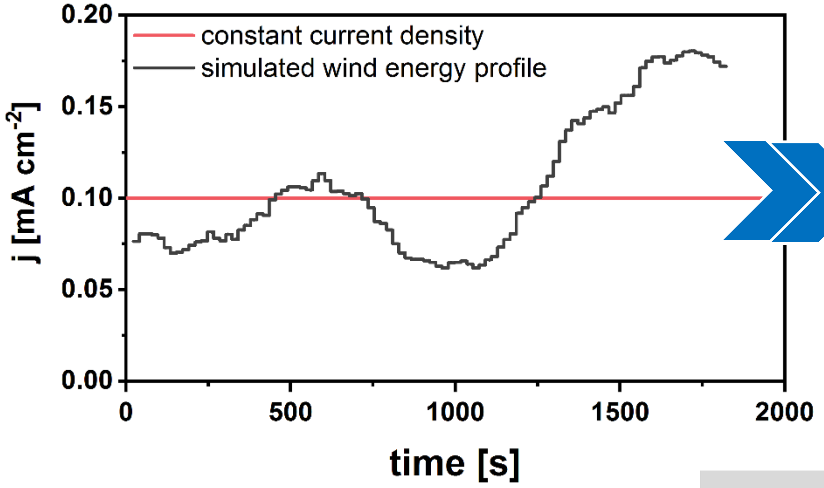
N. Kurig, J. Meyers, E. Richter, S. Palkovits, R. Palkovits, *Chem. Ing. Technik* **2022** 94(5), 786

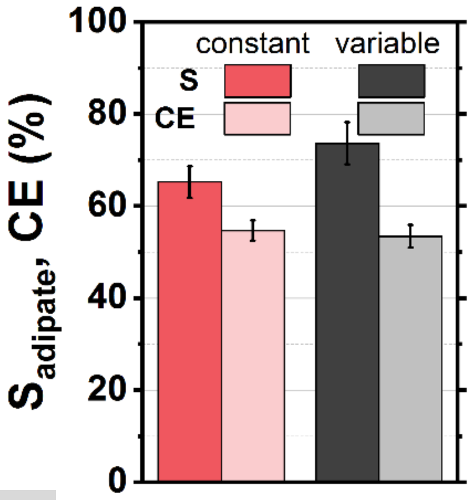


B. Gomes, F. J. Holzhäuser, C. Lobo, P. Ferreira da Silva, E. Danieli, M. Carmo, L. Colnago, S. Palkovits, R. Palkovits, B. Blümich, *ACS Sustain. Chem. Eng.* **2019**, 7, 18288

Dynamic Kolbe Electrolysis of Succinic Acid Ester







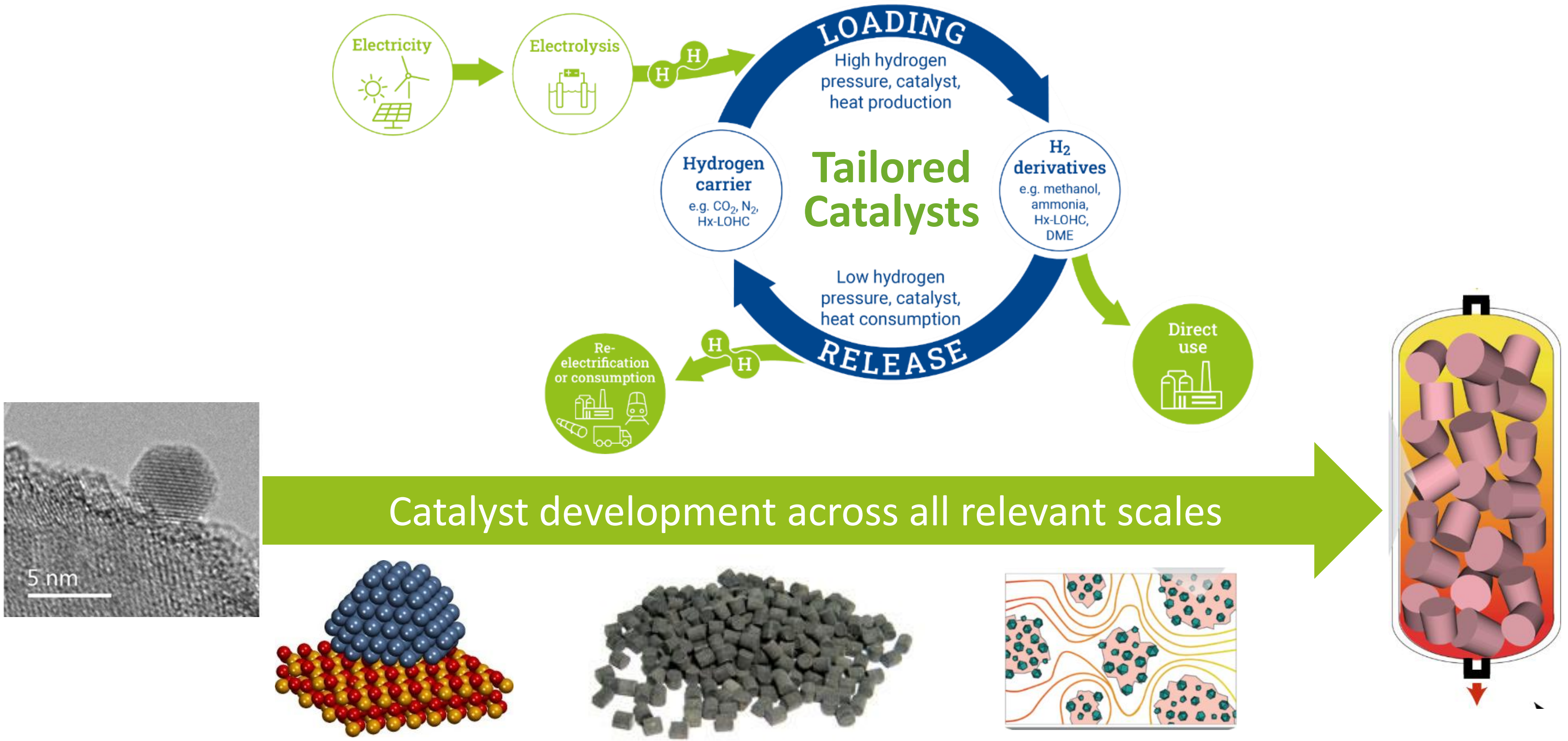
1.0 M HESA
0.1 M NEt_3
100 mA·cm^{-2}

G. Creusen, F. J. Holzhäuser, int. al., R. Palkovits, *ACS Sust. Chem. Eng.* **2018** 6, 17108
N. Kurig, J. Meyers, int. al., R. Palkovits, ACS Sustain. Chem. Eng. **2021**, 9, 3, 1229

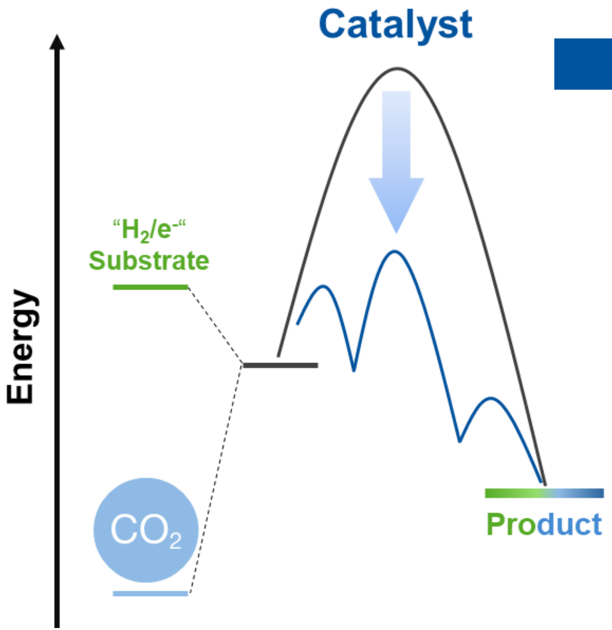
JÜLICH Forschungszentrum RWTH AACHEN UNIVERSITY

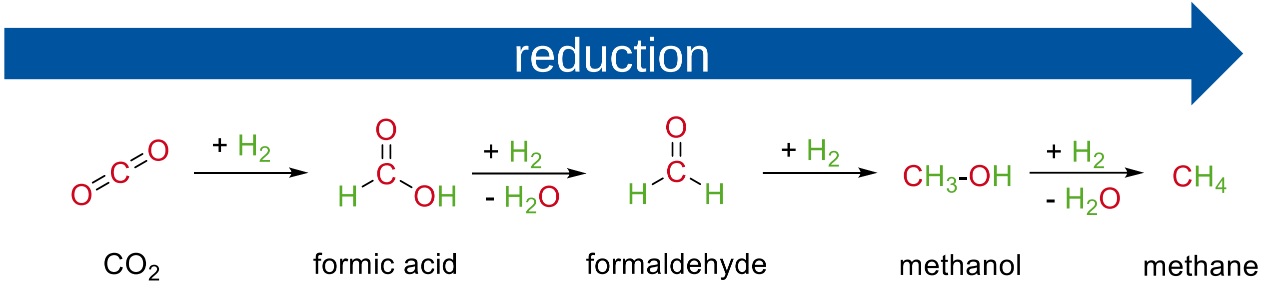
Chemical hydrogen carriers

Enabling long-term storage and long-distance transportation



Hydrogen Storage in C1 Compounds



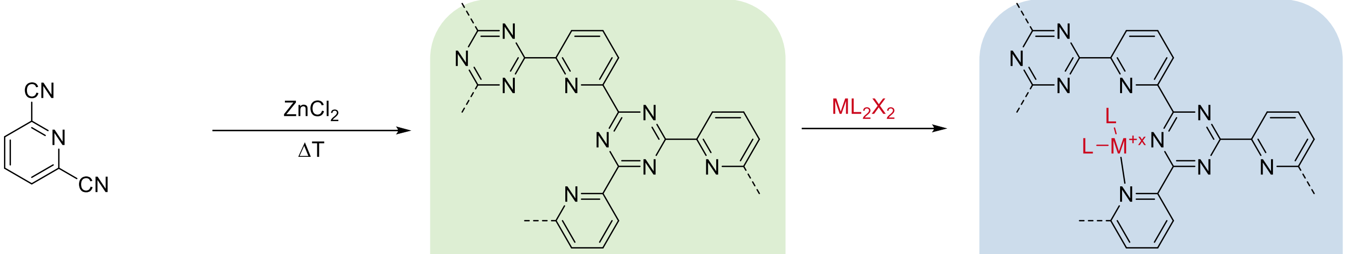


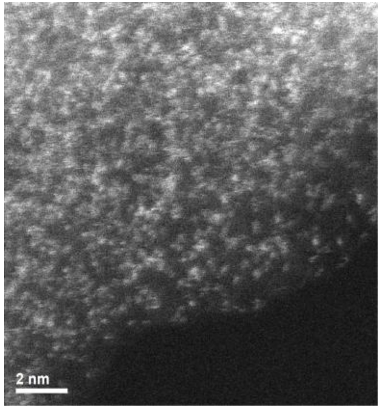
Material Development

Covalent Triazine Framework

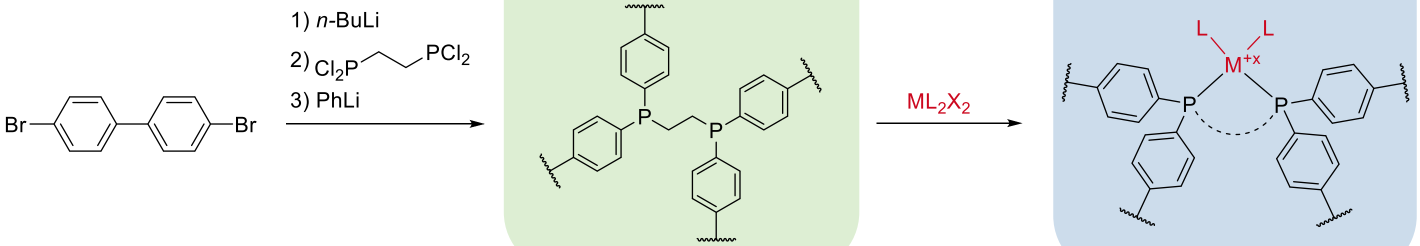
tailored nanoporous polymers

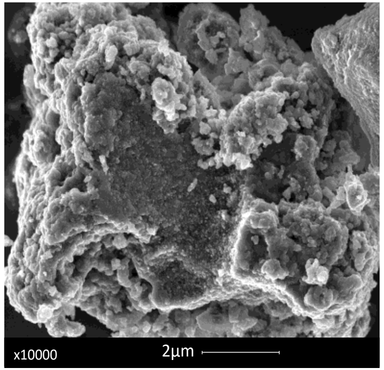
solid molecular catalysts





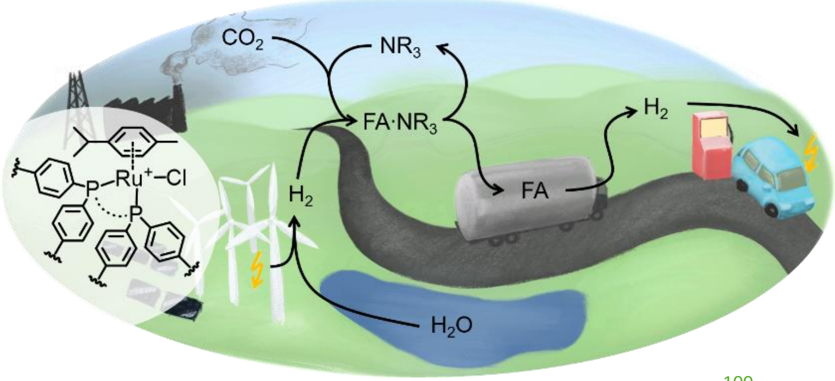
Crosslinked Phosphine Polymers

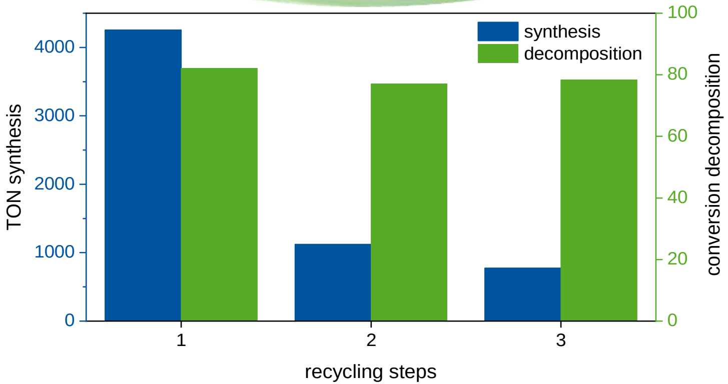




C. Broicher, S. Foit, M. Rose, P. J. C. Hausoul, R. Palkovits, *ACS Catal.* **2017**, 12, 8413
G. Tuci, M. Pilaski, H. Ba, A. Rossin, L. Luconi, S. Caporali, C. Pham-Huu, R. Palkovits and G. Giambastiani, *Adv. Funct. Mater.* **2017**, 27, 1605672
P. J. C. Hausoul, C. Broicher, R. Vegliante, C. Göb, R. Palkovits, *Angew. Chem. Int. Ed.* **2016**, *55*, 5597

Alternating Formic Acid Synthesis & Decomposition: with and without a base

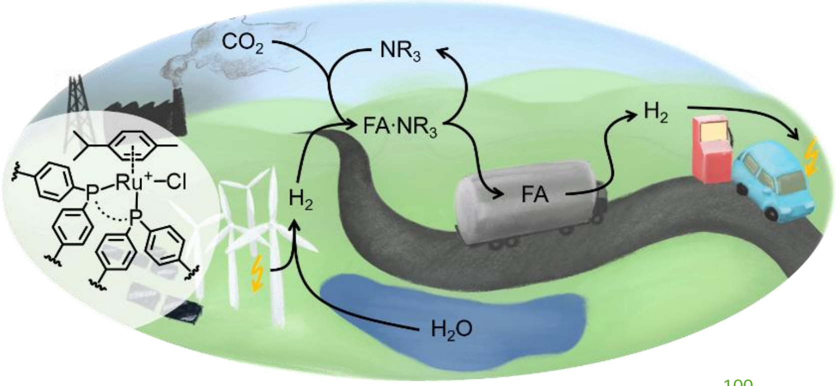


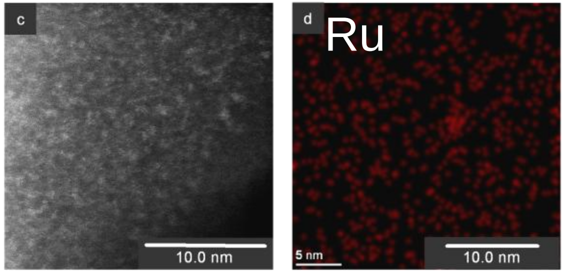


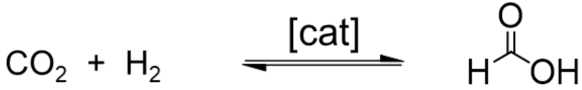
60 vol% aqu. NEt_3, 1wt.% Ru@**P3**; Synthesis: 100 °C, 100 bar CO_2/H_2 (1:1 *v*/*v*), 2 h; Decomposition: 25 mmol FA, 160 °C.

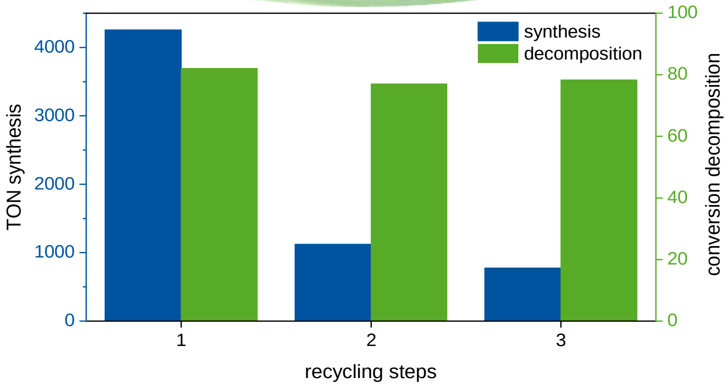
A. Kipshagen, J. Baums, H. Hartmann, A. Besmehn, P. J. C. Hausoul, R. Palkovits, *Catal. Sci. Technol.* **2022**, 12, 5649; J. C. Baums, I. Kappel, A. Meise, P. J. C. Hausoul, M. Heggen, C. Weidenthaler, R. Palkovits, **2025**, submitted

Alternating Formic Acid Synthesis & Decomposition: with and without a base

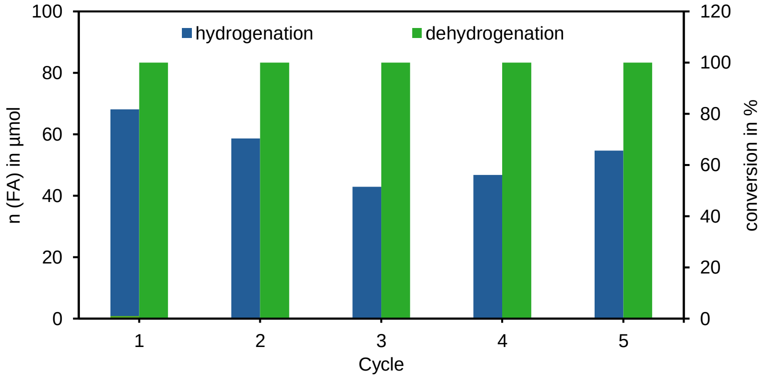








60 vol% aqu. NEt_3, 1wt.% Ru@**P3**; Synthesis: 100 °C, 100 bar CO_2/H_2 (1:1 *v/v*), 2 h; Decomposition: 25 mmol FA, 160 °C.

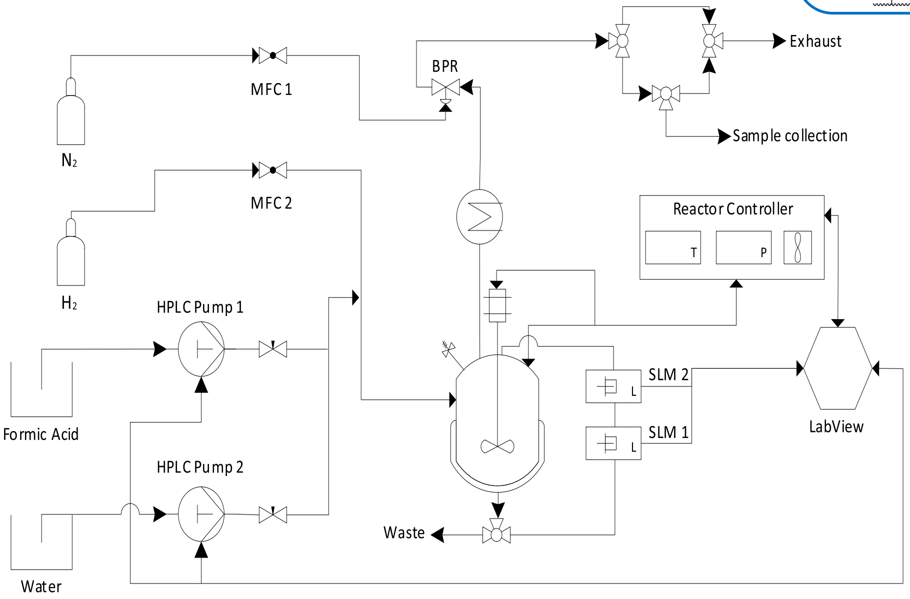


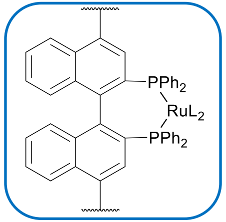
4 mL H_2O, 12 mg catalyst, CO_2/ H_2 (1:1 p/ p, 100 bar), 50 ° C, 18 h. Dehydr.: pressure released, atmosph. flushed with Ar, 160 ° C, 30 min.

A. Kipshagen, J. Baums, H. Hartmann, A. Besmehn, P. J. C. Hausoul, R. Palkovits, *Catal. Sci. Technol.* **2022**, 12, 5649; J. C. Baums, I. Kappel, A. Meise, P. J. C. Hausoul, M. Heggen, C. Weidenthaler, R. Palkovits, **2025**, submitted

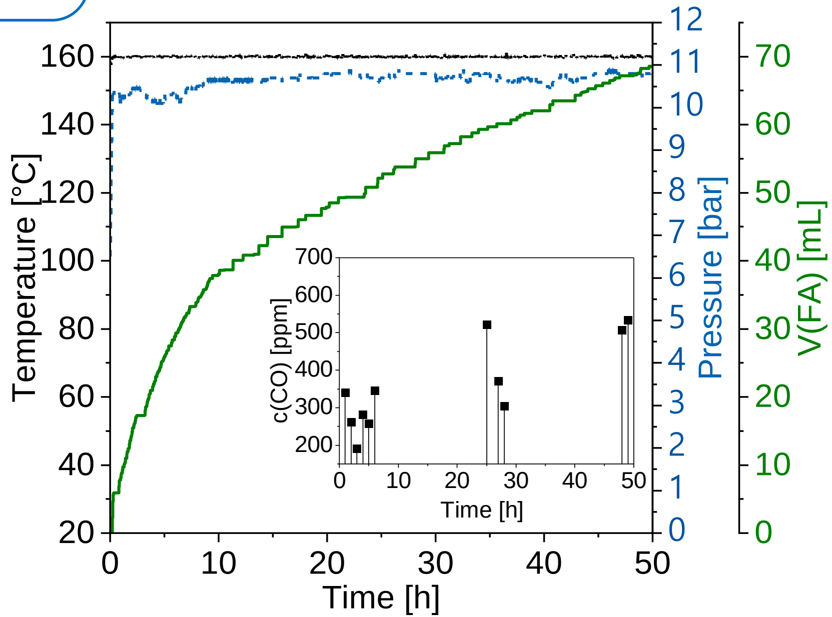
JÜLICH Forschungszentrum
RWTH AACHEN UNIVERSITY

Continuous Operation of Hydrogen Release form Formic Acid





TON of
921.000

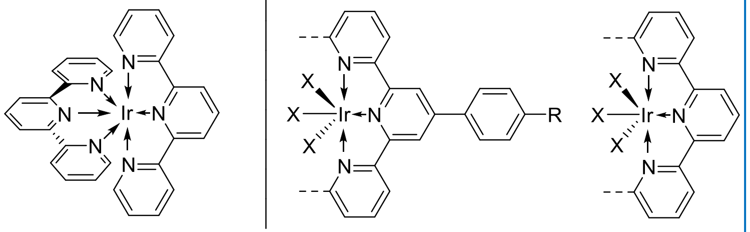


10 wt% aqu. FA, 160°C, 10 bar, 1wt% Ru@Polymer

S. Seidel, I. Kappel, C. Weidenthaler, P. J.C. Hausoul, R. Palkovits, *J. Catal.* **2024** 438, 115712

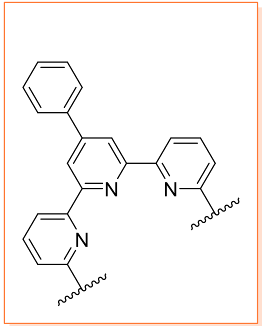
JÜLICH Forschungszentrum RWTHAACHEN UNIVERSITY

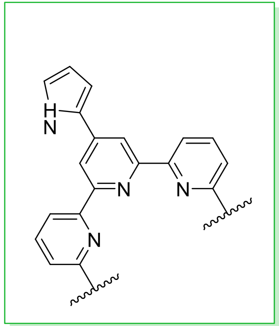
Solid Ir@TerPy Catalyst Platform

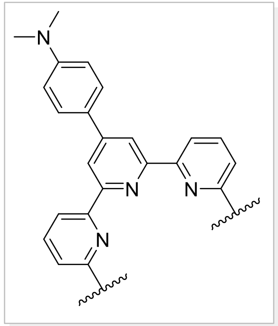


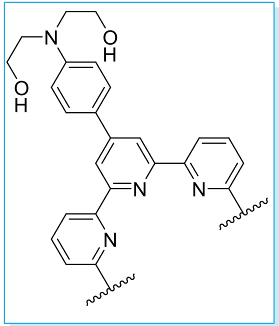
homogeneous bis-terpyridine complex

heterogenized mono-terpyridine complexes with *antenna* interaction

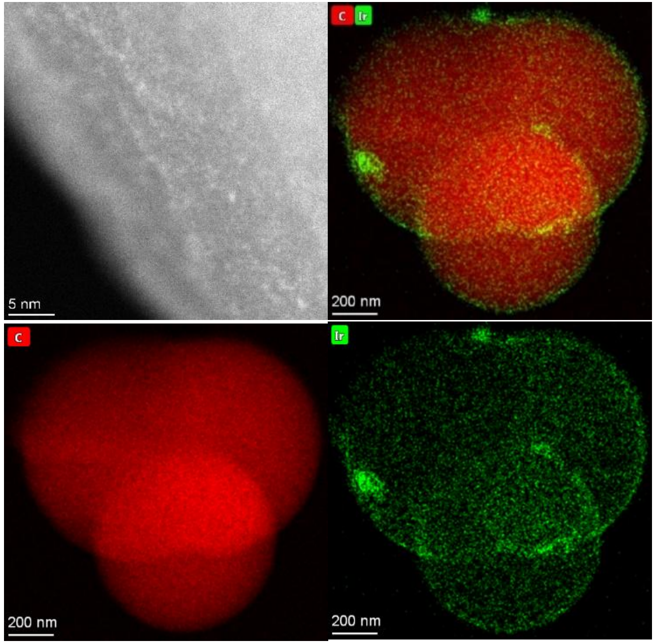








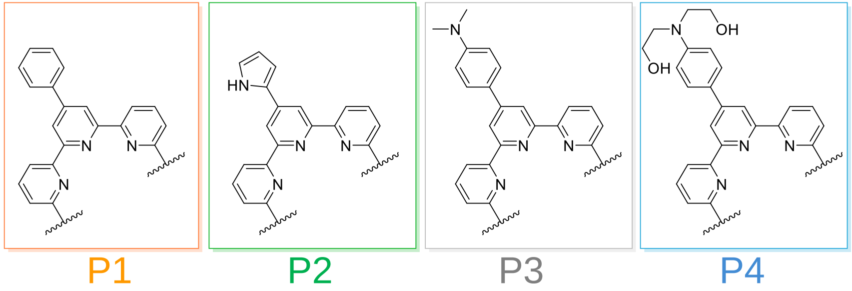
Ir@P2

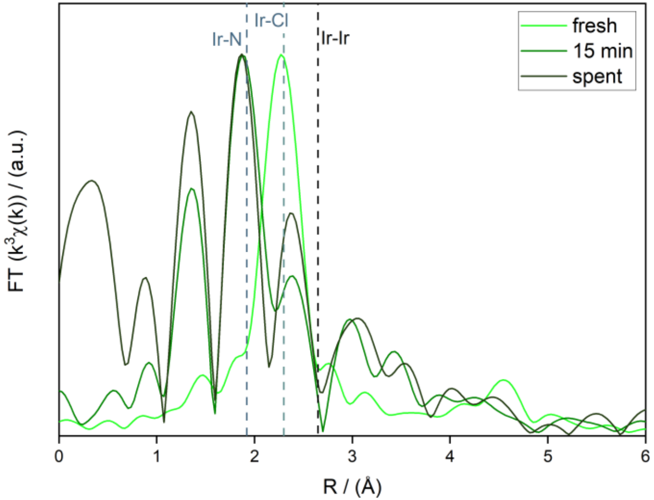


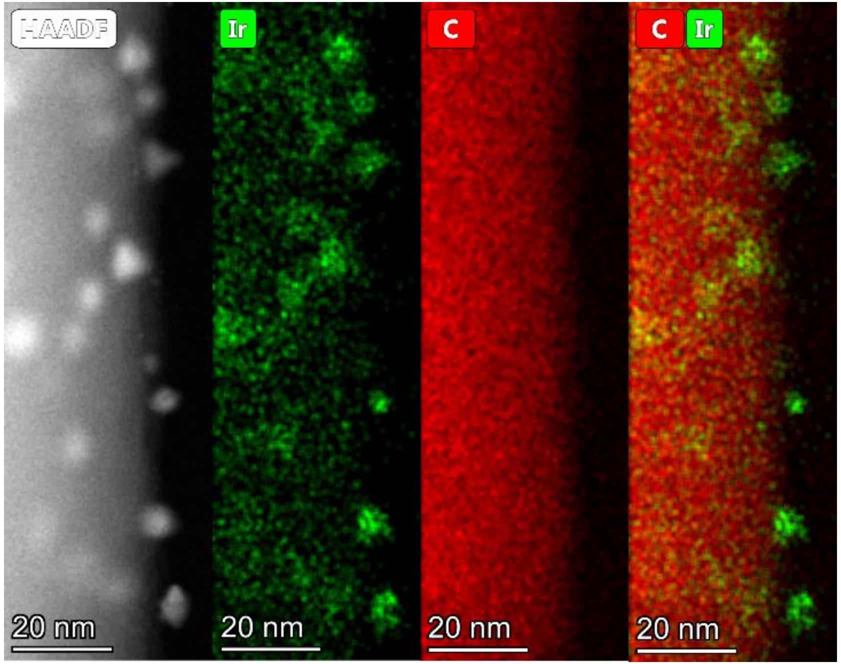
K. Birkelbach, H. Hartmann, A. Besmehn, A. Meledin, I. Kappel, P. J. C. Hausoul, R. Palkovits, **2025**, submitted

JÜLICH Forschungszentrum RWTHAACHEN UNIVERSITY

Solid Ir@TerPy Catalyst Platform



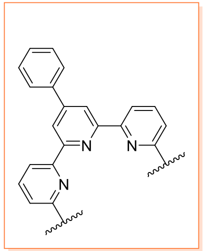




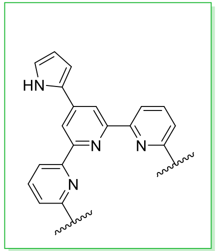
HAADF-STEM image (left) and HAADF-STEM-EDX images (rest) of spent catalyst Ir@P2

K. Birkelbach, H. Hartmann, A. Besmehn, A. Meledin, I. Kappel, P. J. C. Hausoul, R. Palkovits, **2025**, submitted

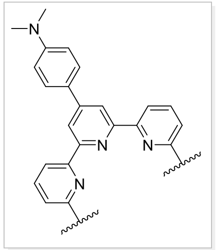
Solid Ir@TerPy Catalyst Platform – Continuous Operation



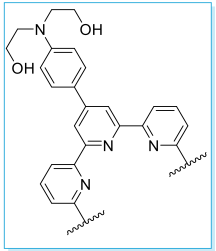
P1



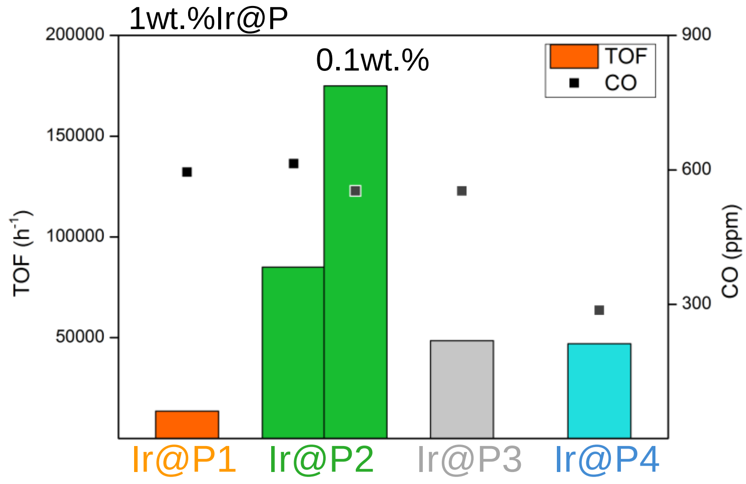
P2



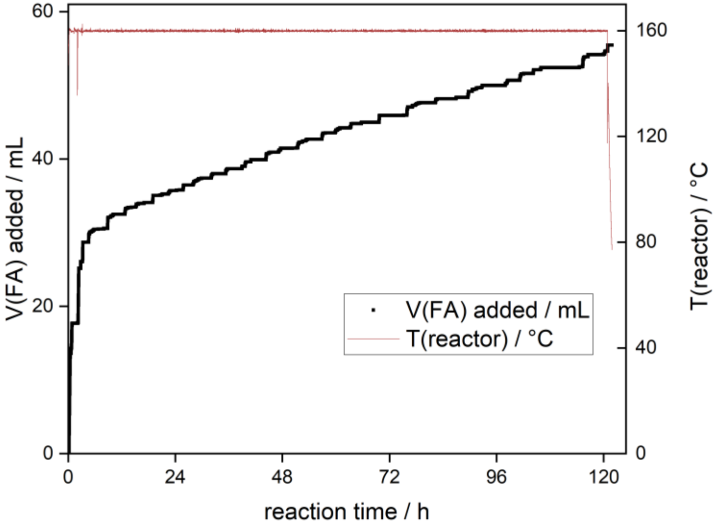
P3



P4



TON of
2 800 000

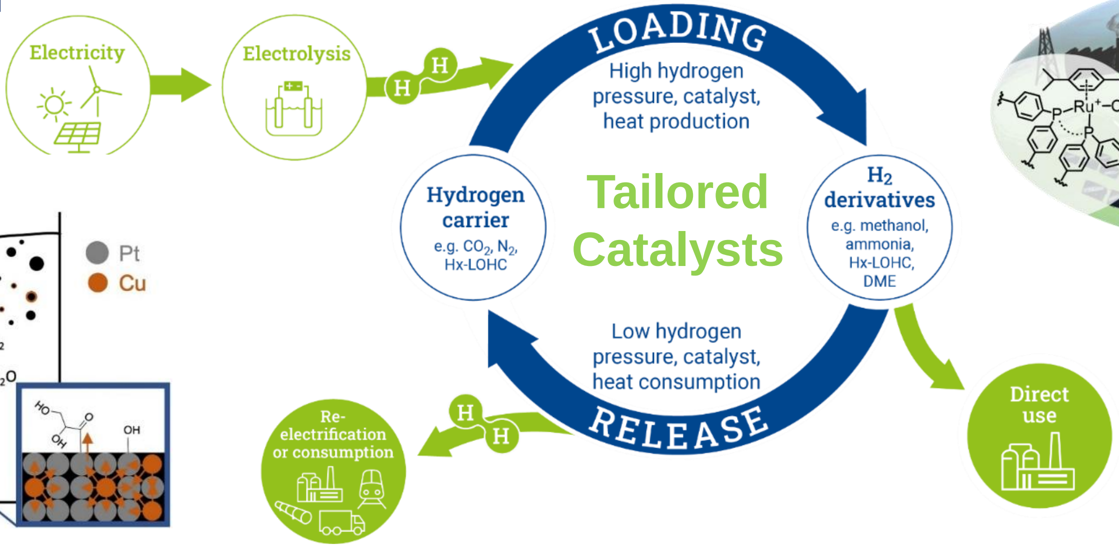


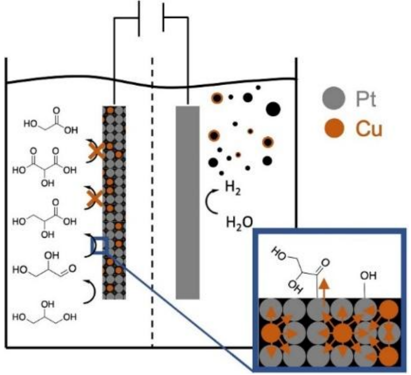
10 wt% aqu. NaOH FA, 160°C, 10 bar, 0.1wt% Ir@P2

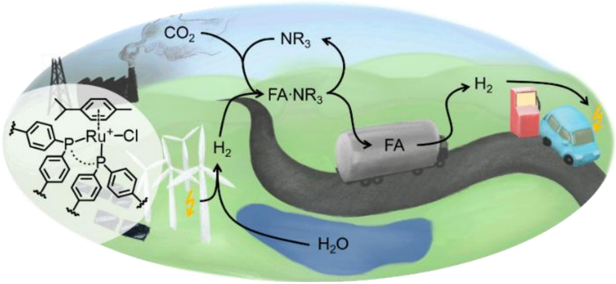
K. Birkelbach, H. Hartmann, A. Besmehn, A. Meledin, I. Kappel, P. J. C. Hausoul, R. Palkovits, **2025**, submitted

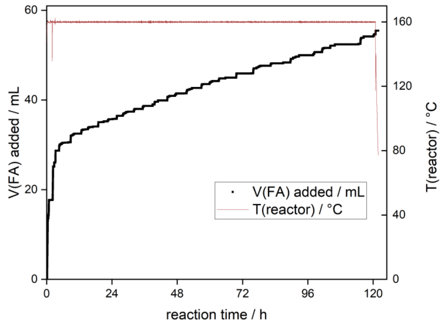
JÜLICH Forschungszentrum RWTH AACHEN UNIVERSITY

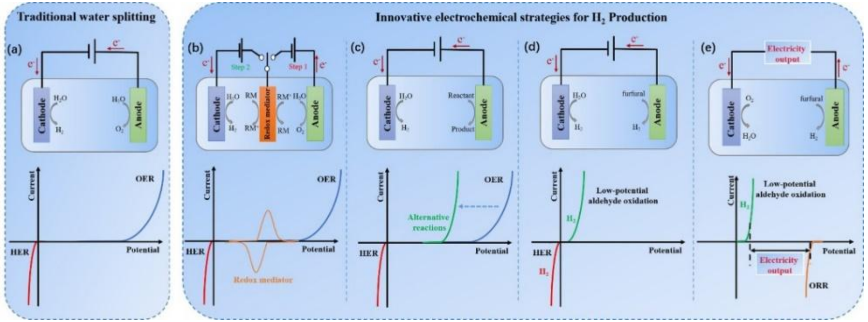
SUMMARY

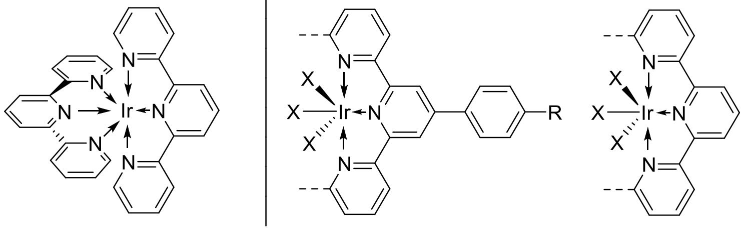












homogeneous bis-terpyridine complex

heterogenized mono-terpyridine complexes with *antenna* interaction

Acknowledgement

“Great things are done by a series of small things brought together”
Vincent Van Gogh

WSS
WERNER SIEMENS-STIFTUNG

catalaix
WSS-Forschungs-zentrum catalaix

FSC The Fuel Science Center

DFG Deutsche Forschungsgemeinschaft

Wasserstoff Leitprojekte
Grün. Groß. Global.

Zukunftscluster Wasserstoff

KOPERNIKUS PROJEKTE
Die Zukunft unserer Energie

NAMOSYN
Nachhaltige Mobilität durch synthetische Kraftstoffe

AUFBRUCH
Graduiertencluster Nachhaltiges Revier

Ministerium für
Kultur und Wissenschaft
des Landes Nordrhein-Westfalen

Ministerium für Wirtschaft,
Industrie, Klimaschutz und Energie
des Landes Nordrhein-Westfalen

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

mpi cec

JÜLICH
Forschungszentrum

RWTH AACHEN UNIVERSITY

Catalyst Design for Efficient Hydrogen Production & Storage in Chemical Hydrogen Carriers

Prof. Dr. Regina Palkovits

r.palkovits@fz-juelich.de
palkovits@itmc.rwth-aachen.de

@PalkovitsLab

Friedrich-Alexander-Universität
Technische Fakultät

Forschungszentrum

Chemical hydrogen storage – systems, challenges and innovations

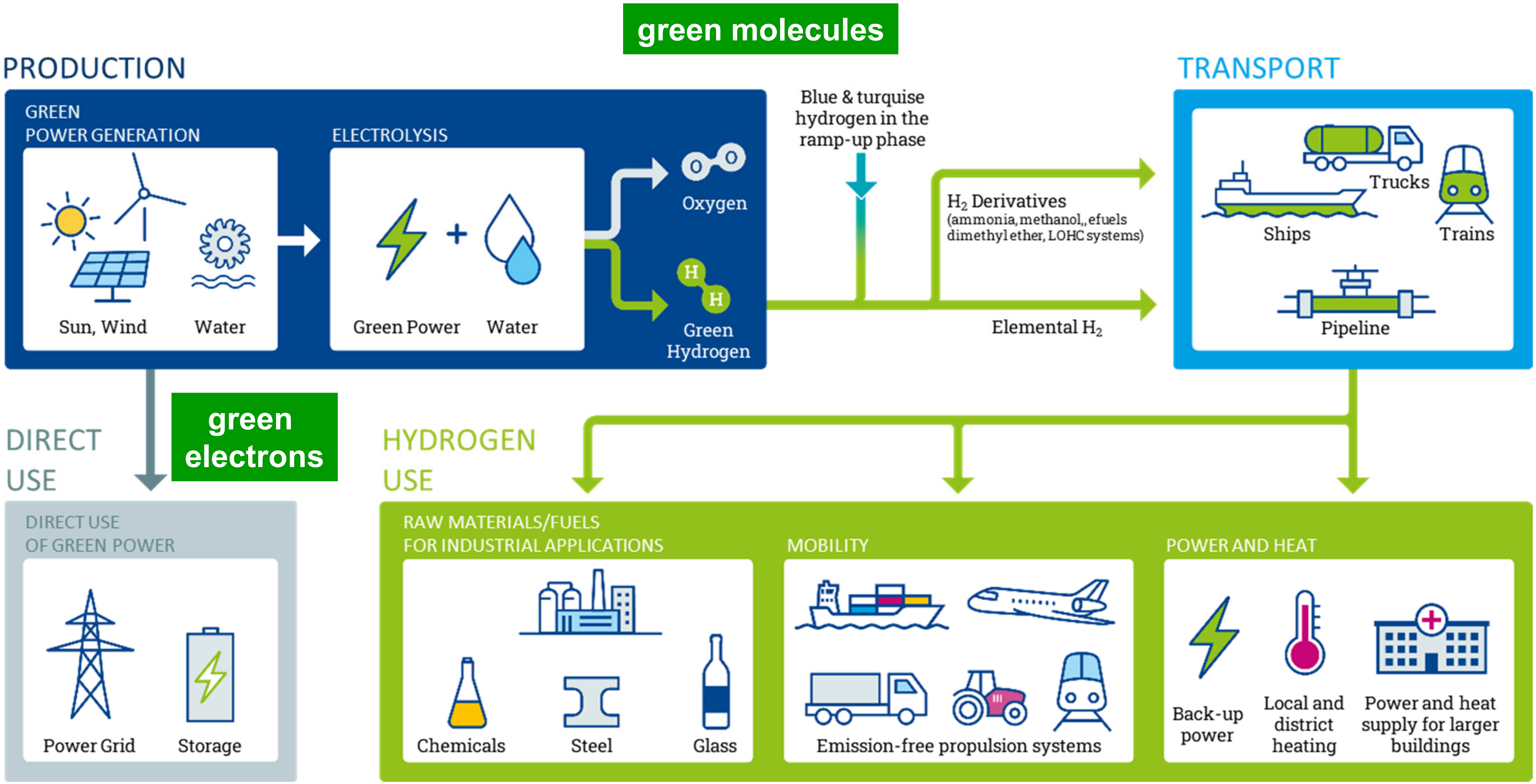
Peter Wasserscheid

Institute for Chemical Reaction Engineering,
Universität Erlangen-Nürnberg

Helmholtz-Institute for Renewable Energies, IET-2 &
Institute for a Sustainable Hydrogen Ecomony (INW)
Forschungszentrum Jülich GmbH

peter.wasserscheid@fau.de
p.wasserscheid@fz-juelich.de

The role of hydrogen in the fully defossilized energy system of the future



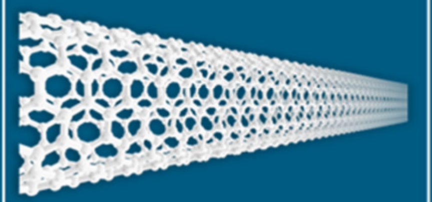
Hydrogen storage and logistics

Advantage: Gravimetric storage density is excellent: **33.3 kWh / kg**

Disadvantage: Volumetric storage density is very low: **3 Wh / L @ 1 bar**

Physical H_2 storage

Adsorptive storage



Metal hydride

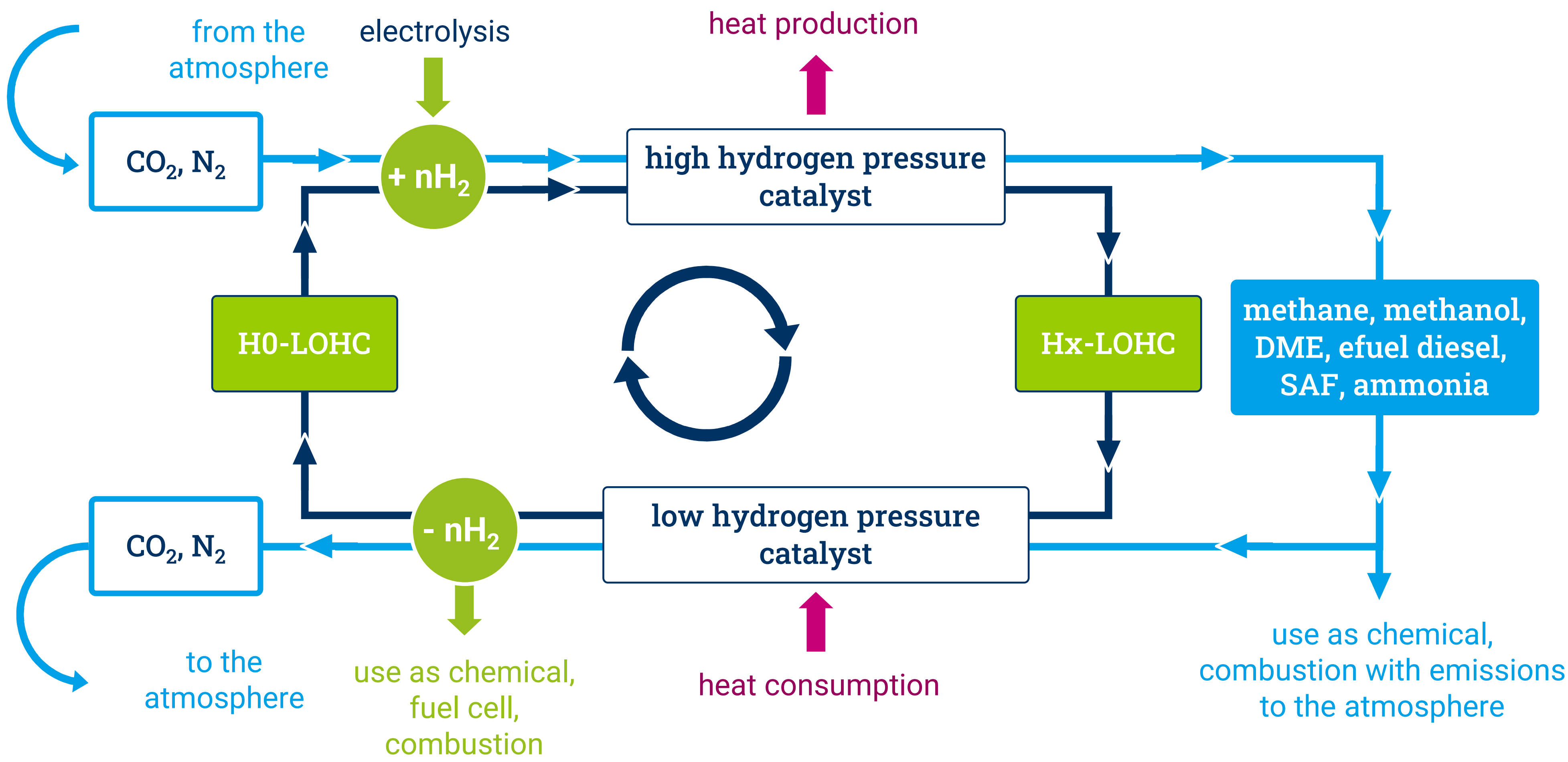
$Na[AlH_4]$

Power-to-X

- Liquid H_2 @ -253 °C
- Compressed H_2 @ 300-700 bar
- Pipeline transport
- Cavern storage

- Hydrogenation of N_2 to NH_3
- Hydrogenation of CO_2 to fuels and chemicals
- Liquid Organic Hydrogen Carrier (LOHC) systems

Chemical hydrogen storage



Chemical hydrogen storage – system characteristics

$CO_2 + x\,H_2 \rightleftharpoons$ methane, methanol, DME, SAF, etc. $+ n\,H_2O$

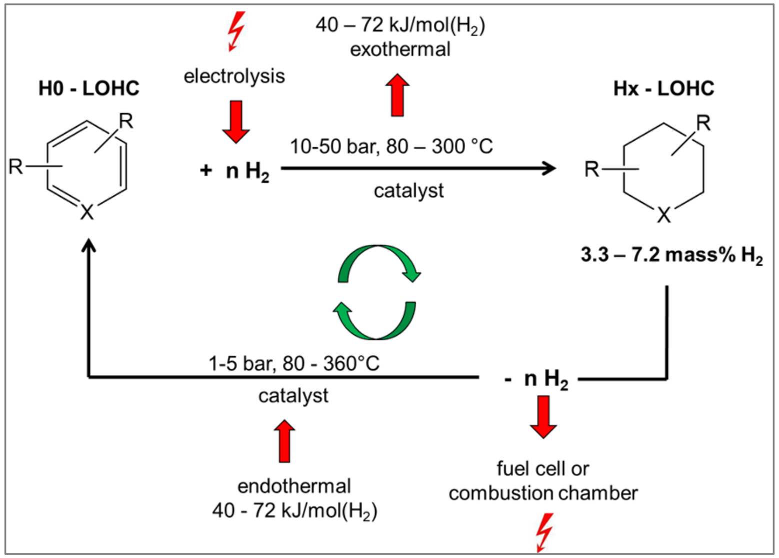
$N_2 + 3/2\,H_2 \rightleftharpoons NH_3$

+ high H_2 capacity
+ moderate reaction enthalphies
+ existing markets for hydrogen. products

- equil.-limited hydrogenation reactions even @ high reaction pressures
- gas mixtures after cracking/reforming
- costly CO_2 extraction from the atmosphere

LOHC technology

H0-LOHC + x H_2 ⇅ Hx-LOHC



- moderate H_2 capacity
- high reaction enthalphies
- no existing markets for hydrogen. products

+ full conversion in hydrogenation reactions even @ low reaction pressures (e.g. 8 bar H_2)
+ pure H_2 after dehydrogenation (> 99.99 %)
+ no gas extraction from the atmosphere

→ we different chemical hydrogen storage technologies !

HELMHOLTZ CLUSTER HYDROGEN (HC-H2)

A MEASURE TO SUPPORT THE STRUCTURAL CHANGE
IN THE RHENISH COAL MINING AREA

PROJECT PERIOD: 2021 – 2038, **TOTAL BUDGET BMBF: 860 M€**
FOUNDING DIRECTOR: PROF. DR. PETER WASSERSCHEID

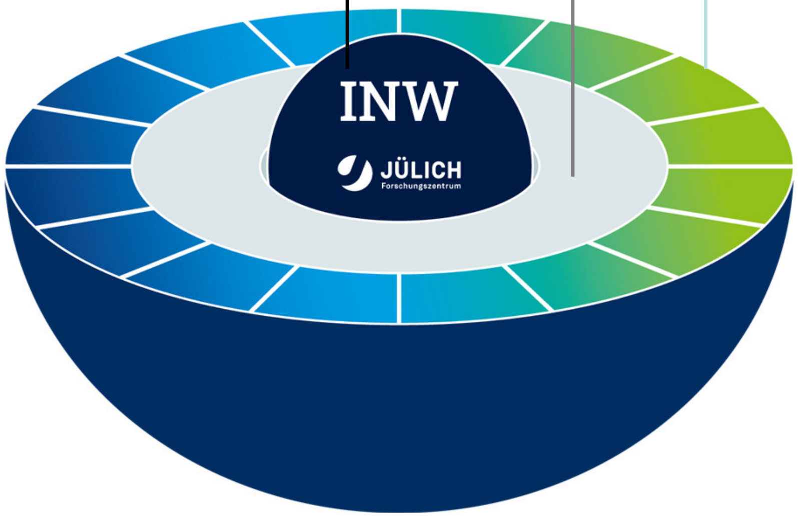
H2 Innovation center = Institute for a sustainable hydrogen economy (INW)

of Forschungszentrum Jülich (FZJ)

Continuity providing core of the HC-H2
located at FZJ

Cooperations with core partners

RWTH Aachen University
FH Aachen
Brainergy Park Jülich



H2 Demonstration region

With partners from industry, academia & municipalities

Innovative demonstrators
10 to 15 plants for innovative **hydrogen technologies** in the Rhenish mining region

Demonstration
of different technological characteristics

Application scenarios and technology aspects
at application-relevant scales

www.hch2.de

funded by Bundesministerium für Bildung und Forschung

Today's menu

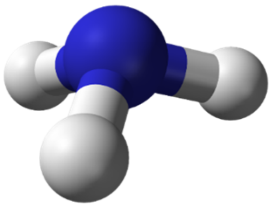
1) H_2-storage using the DME / CO_2 cycle

2) H_2-storage using LOHC systems

Friedrich-Alexander-Universität
Technische Fakultät

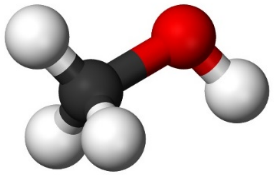
JÜLICH
Forschungszentrum

Hydrogen capacity of CO_2-derived chemical energy storage systems



Ammonia:
Very high hydrogen capacity **(17.7 mass%)**

P. Preuster, A. Alekseev, PW,
Ann. Rev. Chem. Biomol. Eng.,
2017, 8, 445-471.

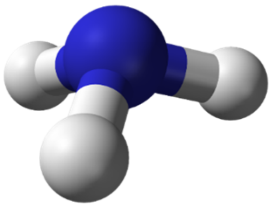


Methanol:
High hydrogen capacity **(12.5 mass%)**

Friedrich-Alexander-Universität
Technische Fakultät

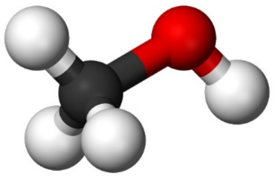
JÜLICH
Forschungszentrum

Hydrogen capacity of CO_2-derived chemical energy storage systems



Ammonia:
Very high hydrogen capacity **(17.7 mass%)**

P. Preuster, A. Alekseev, PW,
Ann. Rev. Chem. Biomol. Eng.,
2017, 8, 445-471.



Methanol:
High hydrogen capacity **(12.5 mass%)**

But is this the technical reality?

$$CH_3OH + H_2O \rightleftharpoons CO_2 + 3\,H_2$$

$M(CH_3OH)$ = 32 g/mol

$M(3\,H_2)$ = 6.0 g/mol

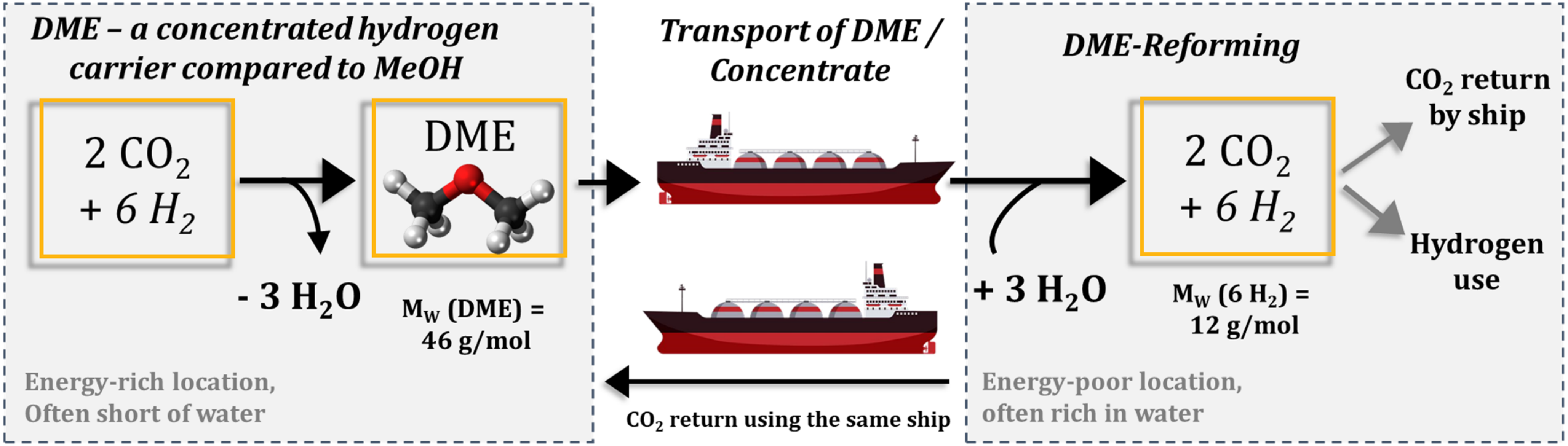
Technical capacity (CH_3OH) = 18.8 mass%

…and what about dimethylether (DME)?

Friedrich-Alexander-Universität
Technische Fakultät

JÜLICH Forschungszentrum

DME as point-to-point hydrogen transport vector – combined with a closed CO_2 loop



Technical hydrogen capacity of DME (mass of deliverd H_2 / mass transported) **= 26.1 %**

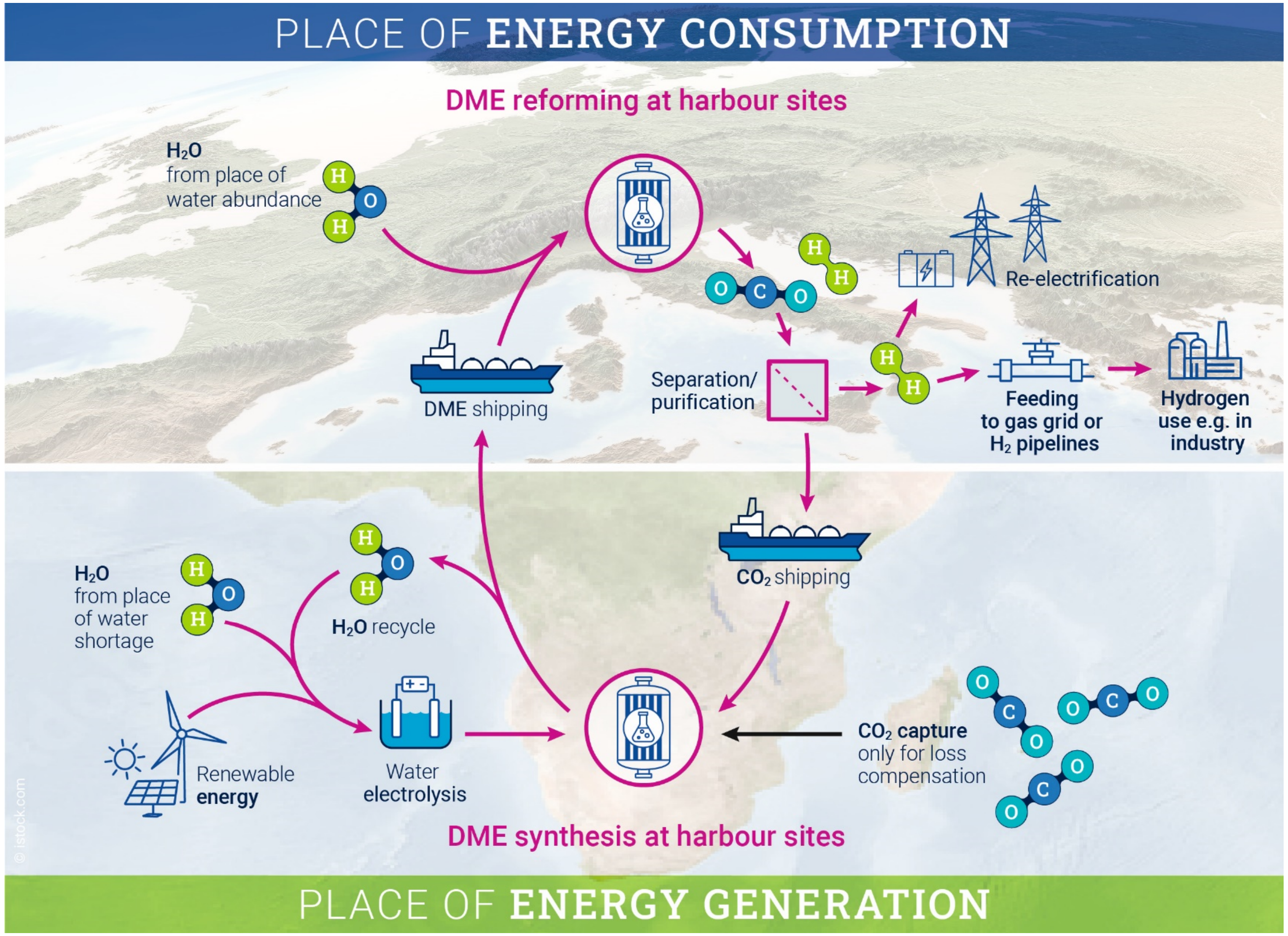
(compared to 17.7.% for NH_3)

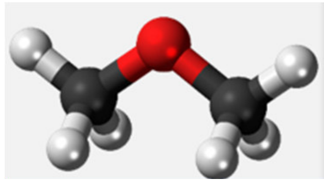
FAU Friedrich-Alexander-Universität Technische Fakultät

JÜLICH Forschungszentrum

Example use case:

H_2 point-to-point delivery Lüderitz (Namibia) - Rotterdam



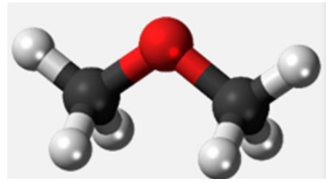


- **Higher hydrogen capacity** and **lower toxicity** compared to ammonia and methanol
- **Closed CO_2 cycle** reduces need for Direct Air Capture of CO_2
- **Much lower water intensity** at the location of renewable energy harvest (- 50% compared to ammonia)

P. Schühle, et int., PW, O. Salem, Energy Environ. Sci., **2023**, DOI: 10.1039/D3EE00228D

Comparison DME *vs.* e-methane

Component	Boiling Point T_{BP}	Liquid density	Viscosity at T_{BP}	LHV	GWP_{100}	Transportation BOG
Dimension	°C	*kg/m³*	*mPa s*	*MJ/kg*	*CO_2 -equiv.*	*%/day*
CO_2	-55 to -50	1178	0.24	-	1	0.12-0.18
DME	-24	735	0.19	28.9	0.3	0.017
CH_4	-162	450	0.12	50	27-30	0.12

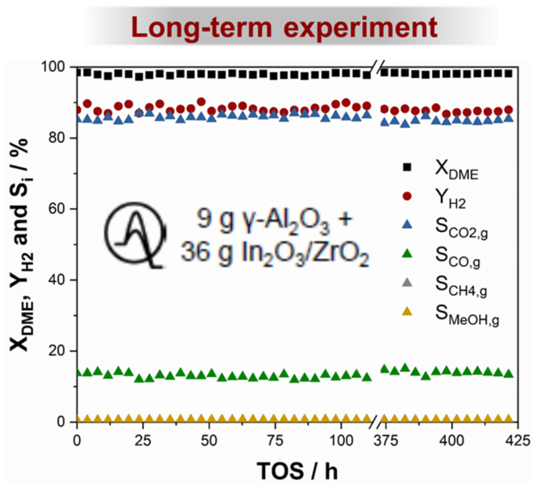


DME and CO_2 have very similar properties → CO_2 back-shipping in the same vessel is possible ! (much easier than for methane / CO_2)

DME has a very low GWP_{100} (*vs.* CH_4) and very low toxicity

Technology readyness:

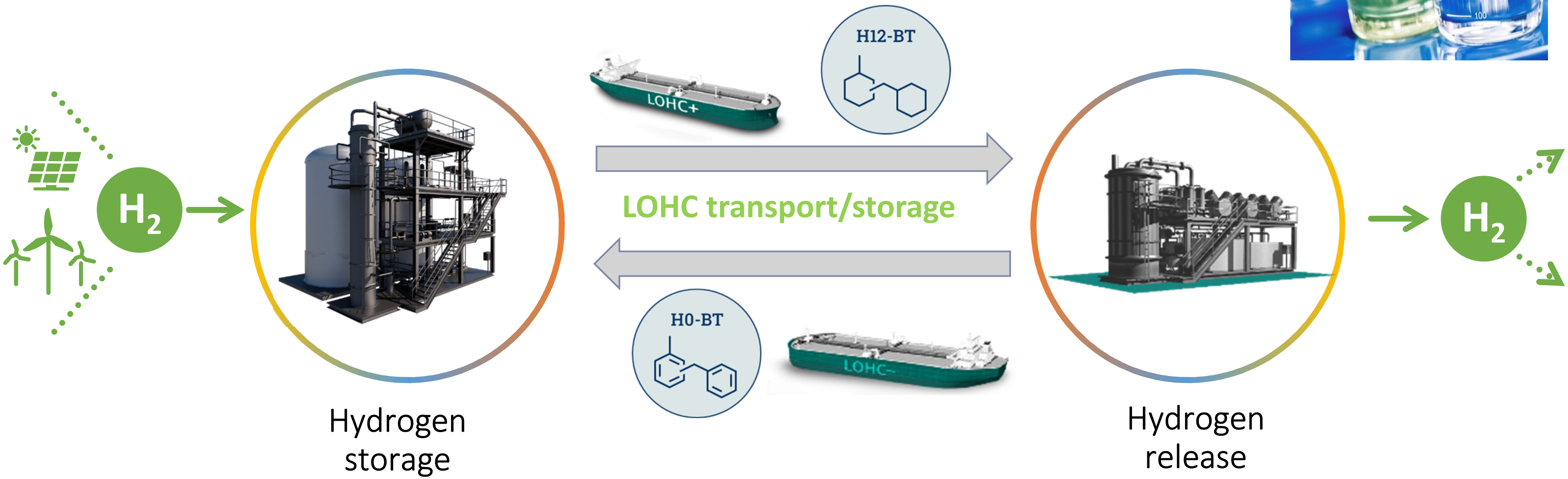
DME synthesis: 8-9
DME shipping: 9
DME reforming: 6-7
CO_2 shipping: 7-8



DME as fuel and potential link for a future sustainable chemicals production:

- DME is a sustainable substitute of propane/butane (if CO_2 is obtained from DAC)
- Most MeOH-to-X processes convert MeOH to DME in the first step: DME opens a route to green ethylene/propylene and polymer production !

2) H_2-storage using LOHC systems



Safe:
LOHC-hydrogen is hardly flammable

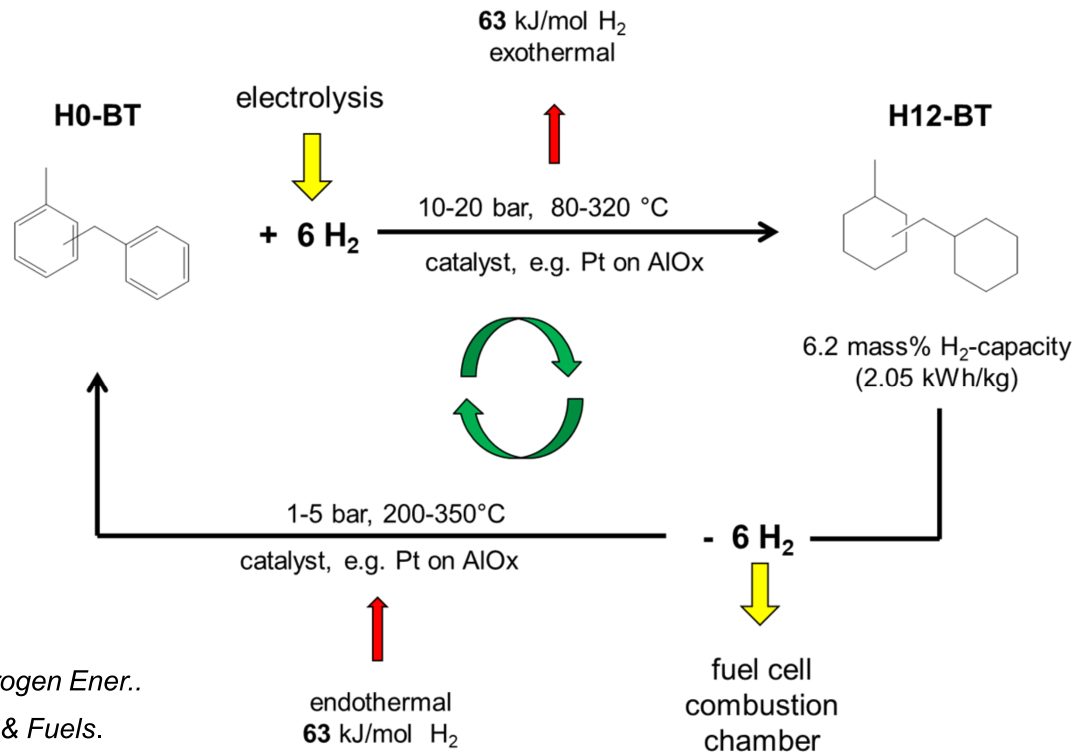
Simple:
Low pressure operations, no extraction/release from/to atmosphere

Flexible:
Storage and transport infrastructure of common fuels can be used

H. Jorschick, P. Preuster, A. Bösmann, PW, Sustainable Energy & Fuels 2021, 5(5), 1311-1346.

Hydrogen storage using the Benzyltoluene-based lohc technology

- Liquid Organic Hydrogen Carrier (LOHC) allow hydrogen storage in fuel-like liquids
- Use of heat transfer fluids established since the 1960s
- LOHC storage compounds are not consumed in the storage cycle
- Charging at moderate pressures; pure hydrogen produced after LOHC condensation



Bulgarin A., Jorschick H., Preuster P., A. Bösmann, P. Wasserscheid (2020), *Int. J. Hydrogen Ener.*.

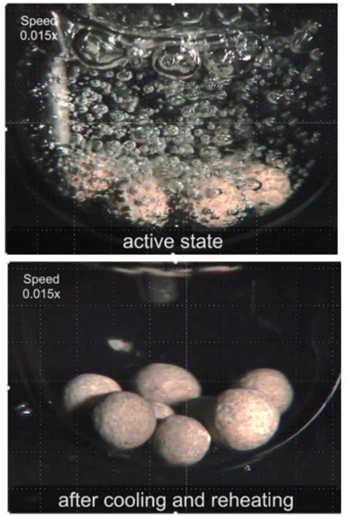
Rüde, R., Dürr S., Preuster P., Wolf M., Wasserscheid P. (2022) *Sustainable Energy & Fuels*.

Willer M., Preuster P., et int., Harting J, Wasserscheid P. (2024) *Int. J. Hydrogen Ener.*

Friedrich-Alexander-Universität
Technische Fakultät

Forschungszentrum JÜLICH

Recent insights and improvements



Bubble nucleation can enhance hydrogen release by a factor of **50**

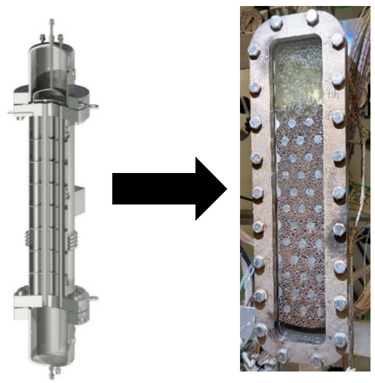
Rate enhancement by bimetallic de-hydrogention catalysts (e.g. Pt/Re)

mm
Catalyst level

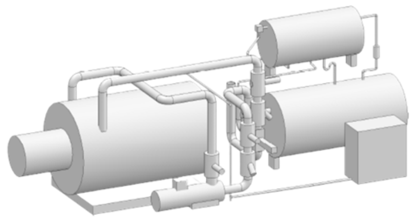
dm
Reactor level

m
System level

Doubling of power density by inversion of fixed-bed reactor



Increase of H_2-system power density by dual reactor concept



D. Strauch, …, J.-D. Grunwaldt, PW, M. Wolf (2024) Catal. Sci. Technol.

T. Solymosi, M. Geißelbrecht, ….N. Vogel, PW (2022). Sci. Adv.

M. Geißelbrecht, S. Mrusek, …A. Bösmann, PW (2020). Energy Environ. Sci.

J: Kadar, F. Gackstatter,… PW, M. Geißelbrecht (2024). Int. J. Hydrogen Ener.

M. Willer, P. Preuster, M. Geißelbrecht, PW (2024). Int. J. Hydrogen Ener.

Patent DE102023200245B3, S. Hahn (2023)

FAU
Friedrich-Alexander-Universität
Technische Fakultät

JÜLICH
Forschungszentrum

Use cases in the mobility sector (benefiting from pure hydrogen release)

H_2 delivery

to large hydrogen filling stations

in operation since 2022

Advantages vs. state-of-the art:

- Cost efficient delivery over long distances
- Cost efficient storage at filling station
- Improved safety at filling station

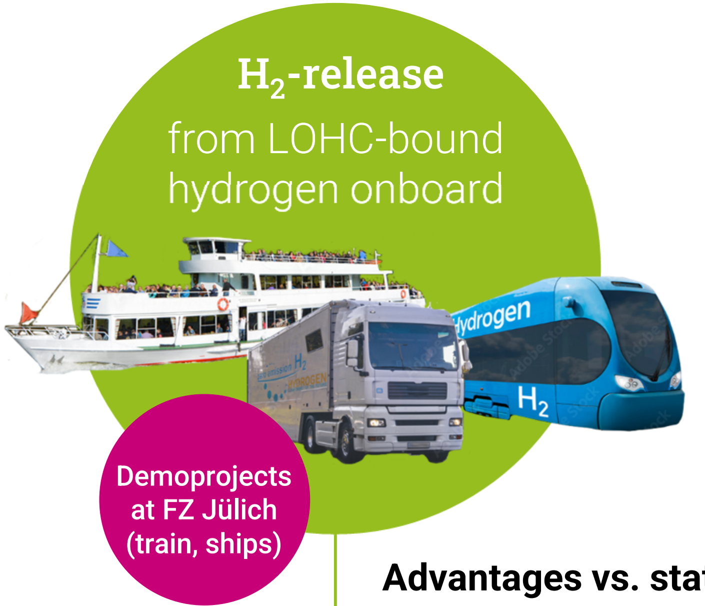
KOPERNIKUS P2X PROJEKTE
Die Zukunft unserer Energie

funded by Bundesministerium für Bildung und Forschung

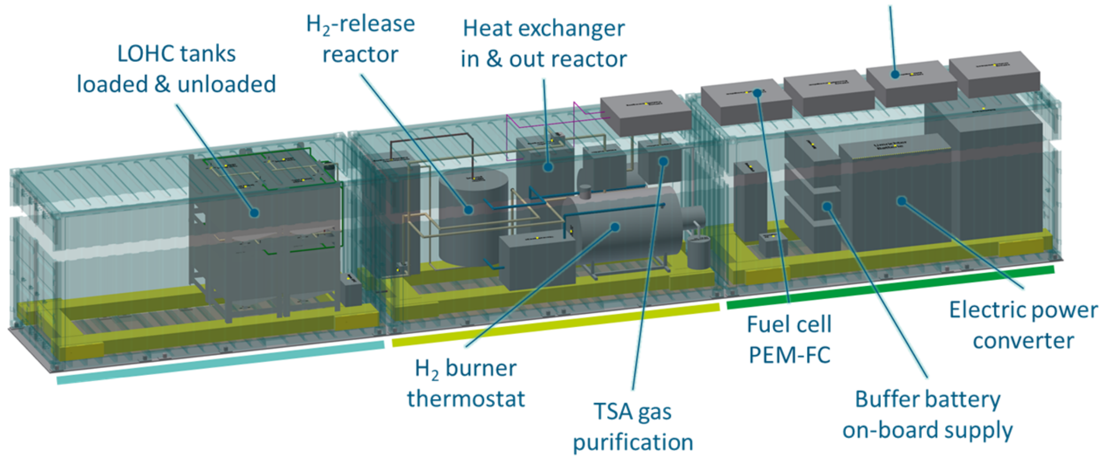
In operation since July 2022:

J. Geiling, ..., P. Wasserscheid, K. Graichen, M. März, P. Preuster, Journal of Energy Storage **2023** ,72, 108478.

Use cases in the mobility sector (benefiting from pure hydrogen release)



800 kW_{therm} power pack design:



M. Willer, …M. Geisselbrecht, PW (2024) Int. J. Hydrogen Ener.

M. Willer, …, J. Harting, PW (2024) Int. J. Hydrogen Ener.

Advantages vs. state-of-the art:

- Use of existing refilling technologies possible
- No need for changing infrastructure beyond vehicle technology
- '*hydrogen-free hydrogen mobility*'

In cooperation with:

SIEMENS

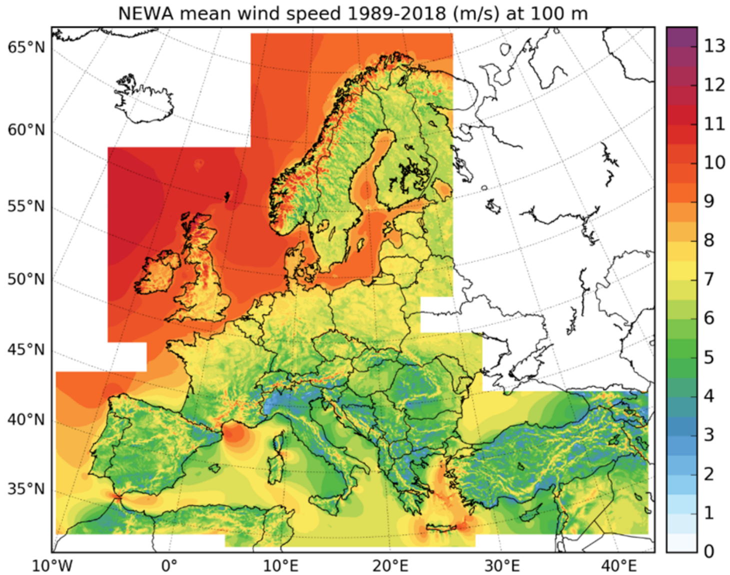
Ingenuity for life

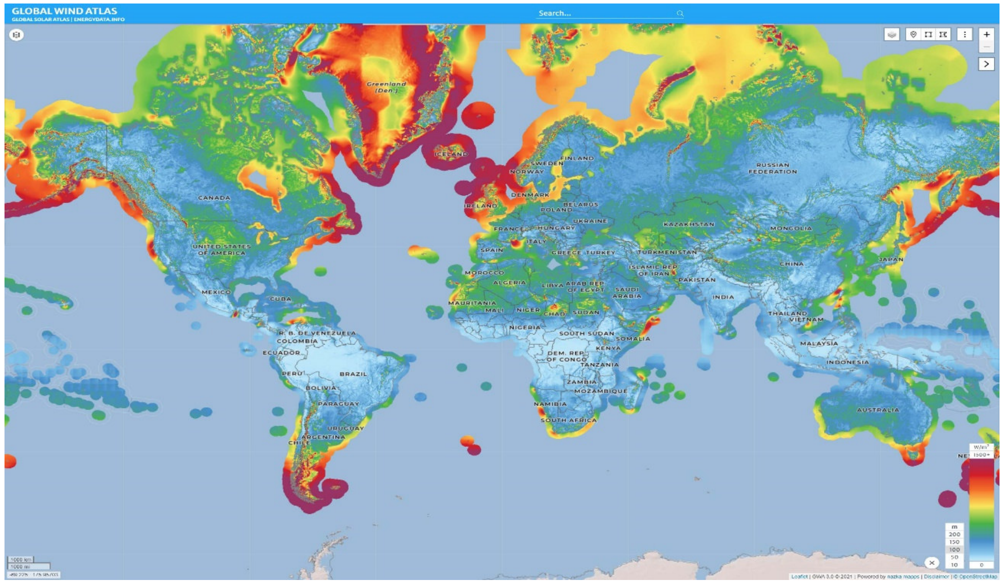
funded by

Bayerisches Staatsministerium für
Wirtschaft, Landesentwicklung und Energie

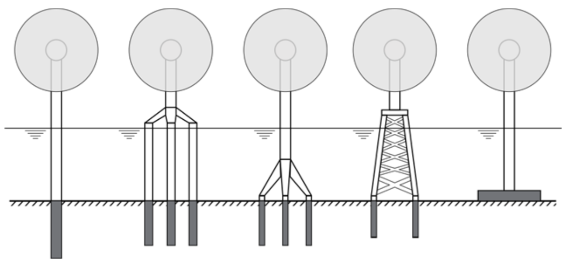
Use cases in energy/hydrogen transportation (benefiting from simple hydrogen storage):

Energy transport from offshore floating wind power installations without land connection

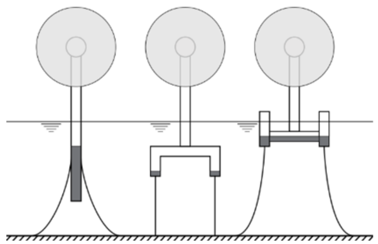




Fixed Foundations (max. 60 m depth)



Floating Substructures:



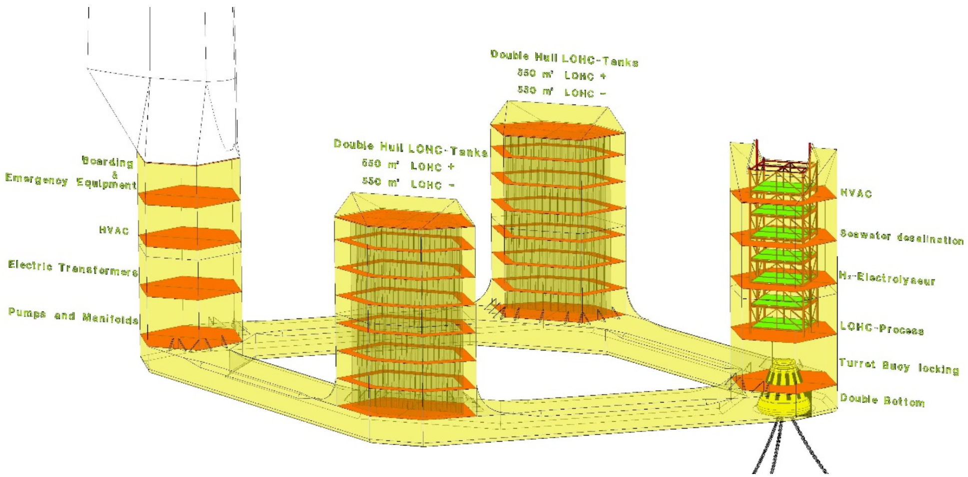
Why shipping green H_2 from wind power from Australia to Korea with excellent wind conditions existing just < 100 miles off the coast in deeper waters ?

Concept: Floating wind power plant with integrated electrolyzer / LOHC charging w/o land connection

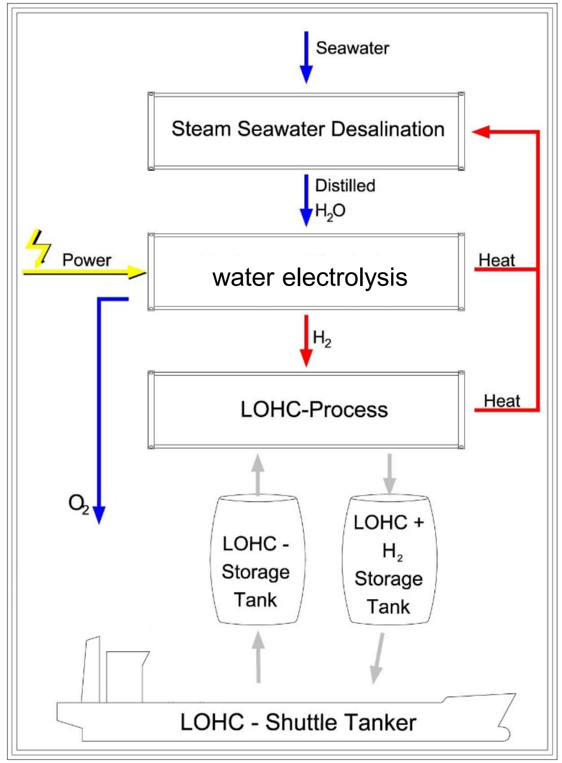
In cooperation with:

TUHH Hamburg University of Technology
CRUSE OFFSHORE GmbH

- 15 MW state-of-the-art wind turbine on floating platform
- Self-adjustment to wind direction



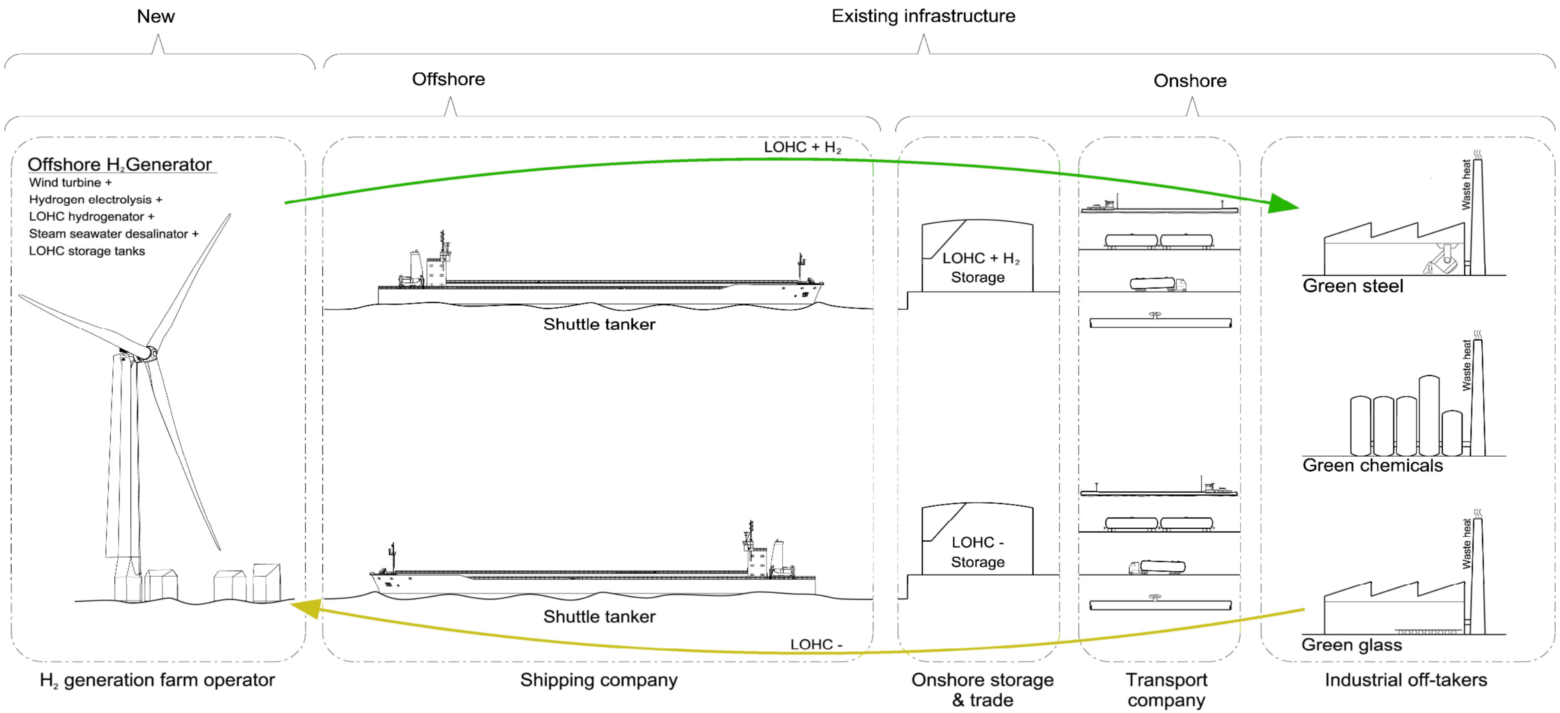
- Water desalination, electrolysis, LOHC hydrogenation and LOHC storage integrated on the platform
- No land connection (no cable, no pipeline)

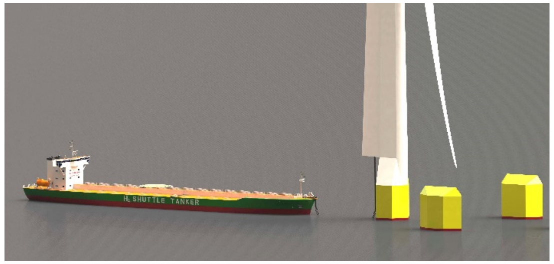


FAU Friedrich-Alexander-Universität
Technische Fakultät

JÜLICH Forschungszentrum

Energy logistics concept





Features:

+ Excellent wind off-shore conditions
+ Short distances to off-taker (very effective use of LOHC carrier)
+ Proven technology from offshore oil/gas industry
+ Moderate investment (reuse of existing assets)
+ Flexility (no connection to land), secured investment


THANK YOU FOR YOUR ATTENTION !

Study of Electrochemical Interfaces and Catalyst Materials for Hydrogen Energy Technology

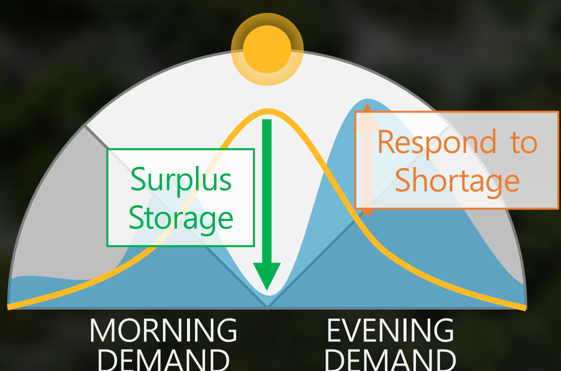
WooChul Jung

The 8th KAST-Leopoldina Bilateral Symposium
Perspectives on Energy Transition, 2025.01.14

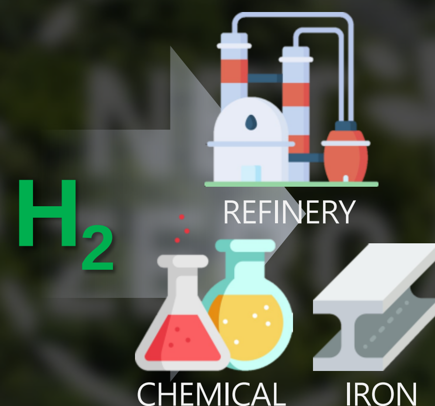
Hydrogen Energy Technology

Key for Achieving Net Zero 2050 !

Why Green Hydrogen?



Addressing Renewable Energy Instability



Achieving Carbon Reduction in Industry

Being Utilized for Green Energy Generation

Examples of the Importance of Hydrogen

Industrial Applications and Transportation

Steel Industry

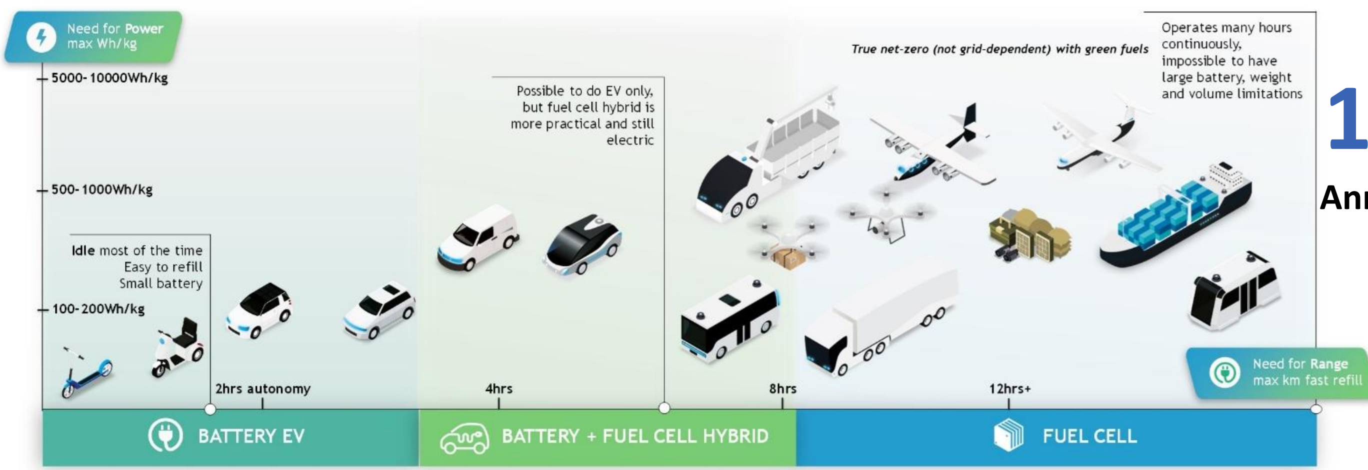
POSCO

$ 31 Billion by 2050

Investment on conversion to HyREX(hydrogen reduction) Steel

*** Green hydrogen as a feedstock to produce Direct Reduced Iron(DRI)**

Transportation



1 Billion Tons

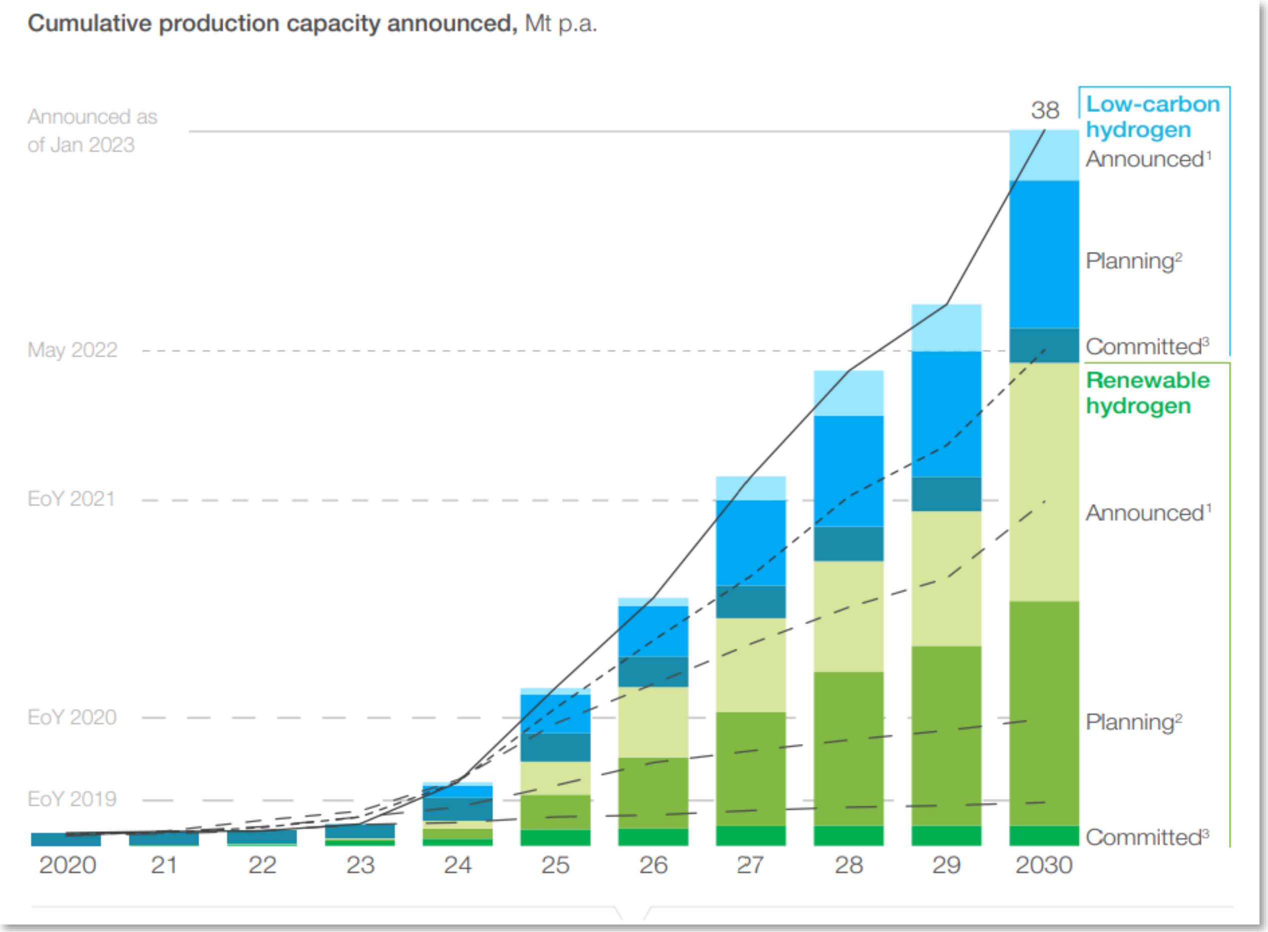
Annual Greenhouse Gas Emissions from Ships

Powertrain Decarbonization by Green Hydrogen

Worldwide Hydrogen Demand

Hydrogen Production Scenario

Based on sum of current policies of each country, production is expected to be 250 Mt by 2050.



By 2030,

210 Mt

Demand to meet NetZero 2050

110 Mt

Announced Global Demand

38 Mt

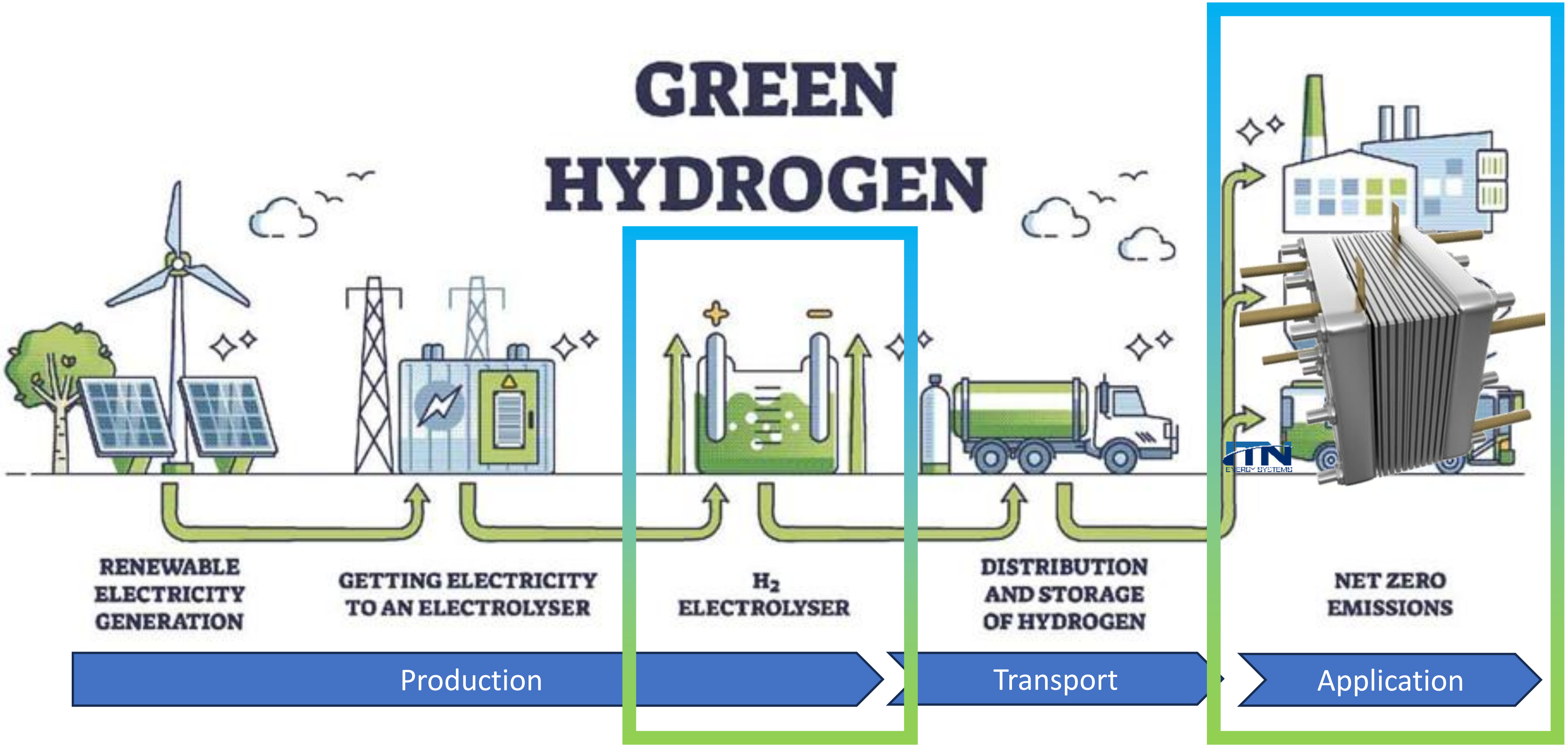
Announced Global Production

Only 34% in progress

Hydrogen Council, McKinsey & Company, *Hydrogen Insights 2023*

Production, Transport, and Application

Our group's Target Applications



Water Electrolysis Cells

Reformers

Fuel Cells

Main Applications of Interest

Solid Oxide Electrolysis Cell (SOEC)

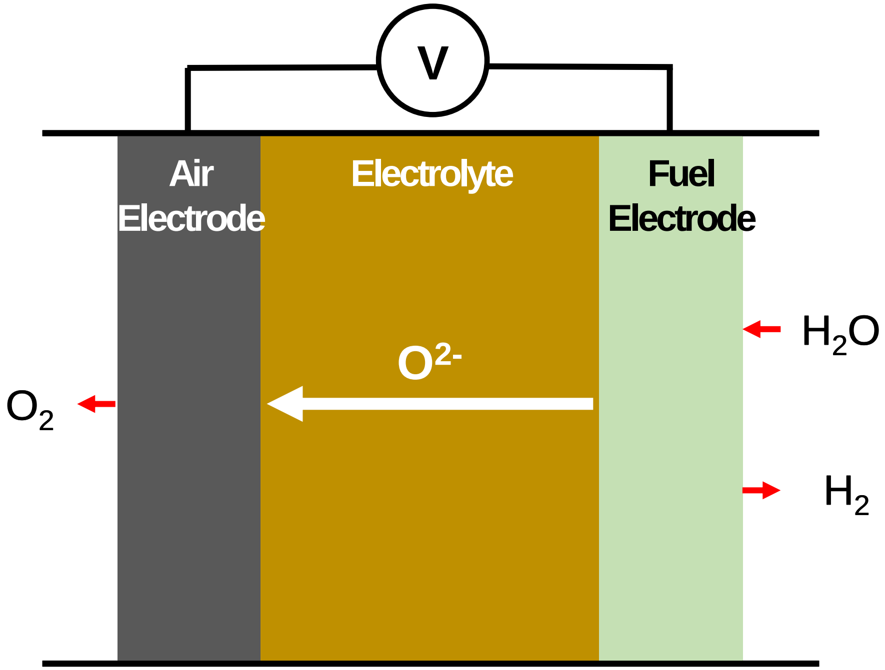
$$H_2O + 2e^- \rightarrow H_2 + O^{2-}$$

$$2O^{2-} \rightarrow O_2 + 4e^-$$

$$CO_2 + 2e^- \rightarrow CO + O^{2-}$$

$$N_2 + 6H^+ + 6e^- \rightarrow 2NH_3$$

$$C_2H_6 \rightarrow C_2H_4 + 2H^+ + 2e^-$$



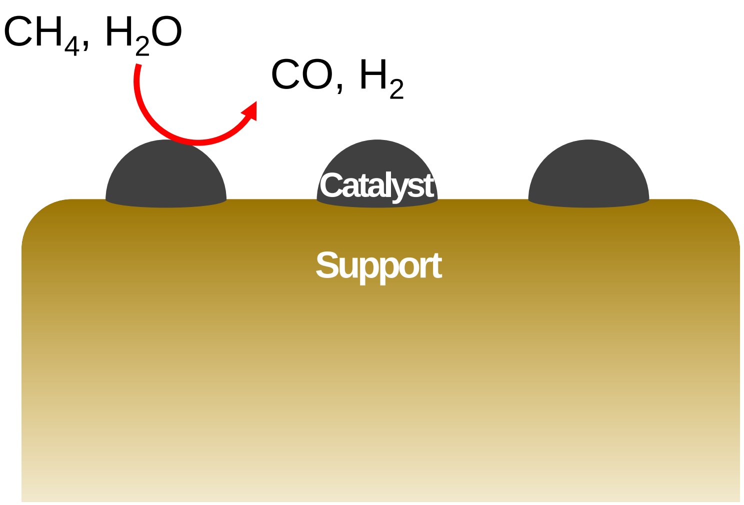
Reformer for Hydrogen Production

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

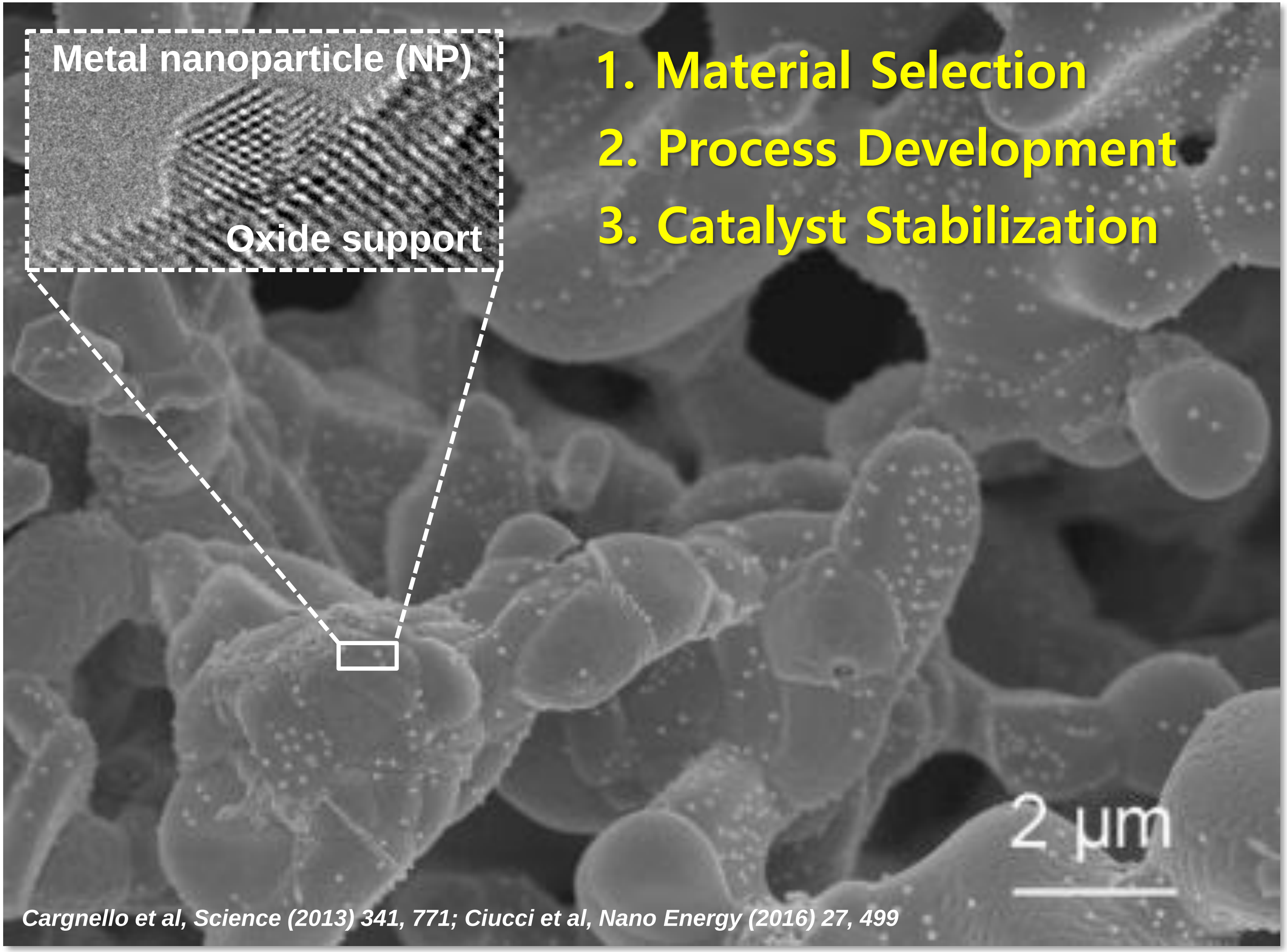
$$CH_4 + CO_2 \rightarrow 2CO + 2H_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

$$2NH_3 \rightarrow N_2 + 3H_2$$



Supported Catalyst and Electrode Materials



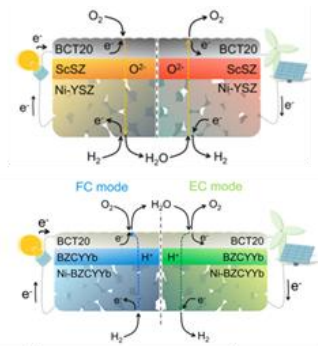
Cargnello et al, Science (2013) 341, 771; Ciucci et al, Nano Energy (2016) 27, 499

1. Ceramic Electrode Materials & Processing

Designing Advanced Materials with High Performance/Durability

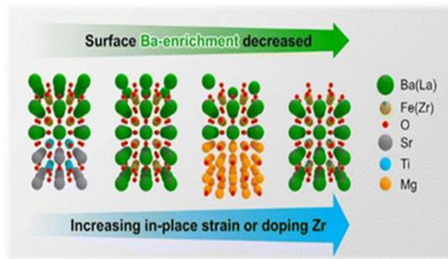
Development of Universal Electrode Materials

Stabilizing BCO *via* Ta-doping ($BaCo_{1-x}Ta_xO_{3-d}$)



Energy Environ. Sci. 16 (2023) 3803

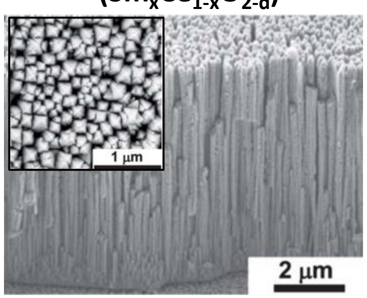
Stabilizing BLF *via* Zr-doping ($Ba_{0.95}La_{0.05}Fe_{1-x}Zr_xO_{3-d}$)



Energy Environ. Sci. 15 (2022) 4069

Development of Ceria-based Electrode Materials

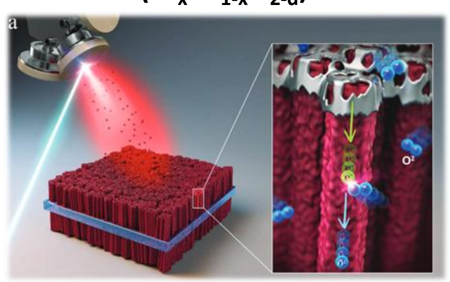
Activating CeO_2-based fuel electrode *via* Sm-doping ($Sm_xCe_{1-x}O_{2-d}$)



Energy Environ. Sci. 5 (2012) 8682

Energy Environ. Sci. 7 (2014) 1685

Activating CeO_2-based fuel electrode *via* Pr-doping ($Pr_xCe_{1-x}O_{2-d}$)



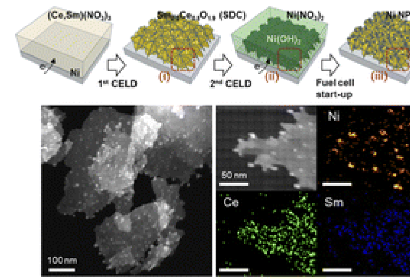
Advanced Energy Materials 12 (2022) 2202101

Advanced Energy Materials 8 (2018) 1703647

Designing Fabrication Technique for Nanocomposite Electrodes

Electrode Activation *via* Electrochemical Deposition

Performance improvement *via* applying active catalyst

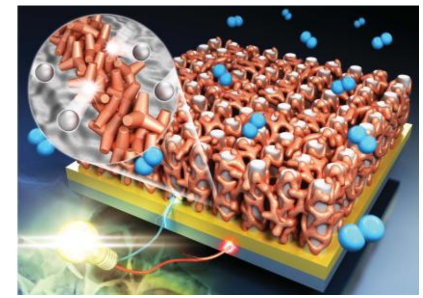


Advanced Materials (in revision)

JMCA 10 (2022) 20886

JMCA 4 (2016) 9394

Stabilization *via* highly stable oxide coating



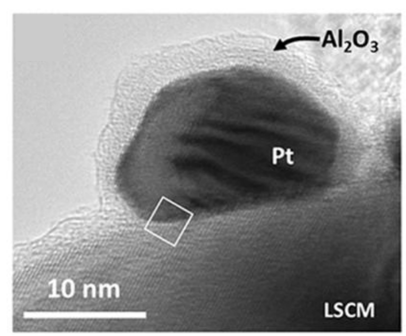
JMCA 8 (2020) 14491

Advanced Energy Materials 8 (2018) 1703647

Nano Energy 23 (2016) 161

Design of Composite Electrodes *via* ALD

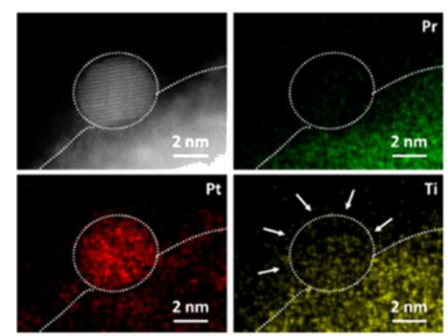
Nanocomposite electrode with oxide overcoating



Chem. Eng. J. 455 (2023) 140611

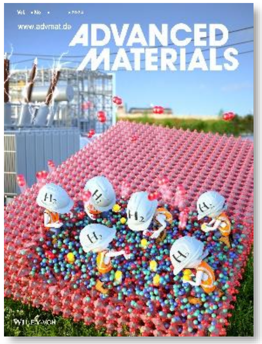
ACS AMI 12 (2020) 4405

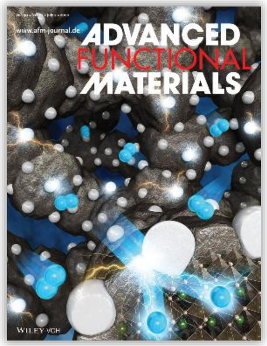
Nanocomposite electrode with oxide undercoating

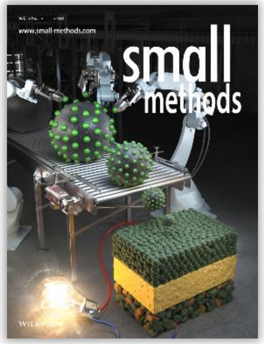


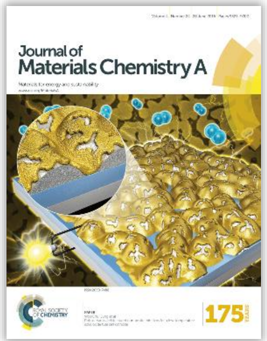
ACS Catalysis 12 (2022) 8593

1. Ceramic Electrode Materials & Processing







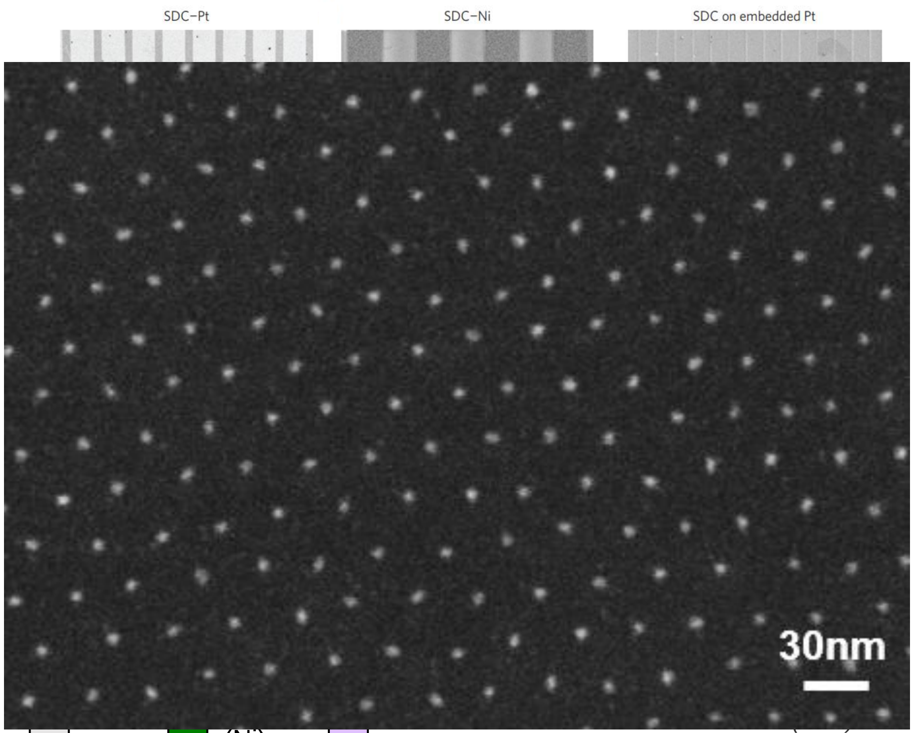


Adv. Mater. (2024) IF = 29.4	Energy Environ. Sci. (2023) IF = 32.5	Adv. Energy Mater. (2022) IF = 27.8	Adv. Funct. Mater. (2022) IF = 19.92	Small Methods (2023) IF = 12.4	J. Chem. Eng. (2023) IF = 16.74
ACS Catalysis (2022) IF = 13.7	ACS Nano (2022) IF = 18.03	Energy Environ. Sci. (2022) IF = 32.5	J. Mater. Chem. A (2022) IF = 11.9	J. Mater. Chem. A (2022) IF = 11.9	J. Mater. Chem. A (2022) IF = 11.9
Nanoscale Advances (2022) IF = 5.598	ACS AMI (2020) IF = 9.5	Electrochimica Acta (2019) IF = 7.336	J. Alloys Compd. (2019) IF = 6.371	Adv. Energy Mater. (2018) IF = 27.8	Nature Comm. (2018) IF = 16.6
Ceram. Int. (2018) IF = 5.532	J. Power Sources (2017) IF = 9.794	Nano Energy (2016) IF = 19.07	J. Mater. Chem. A (2016) IF = 11.9	Energy Environ. Sci. (2014) IF = 32.5	Energy Environ. Sci. (2012) IF = 32.5

28 related articles have been published.

2. Model System Study with Well-defined Interfaces

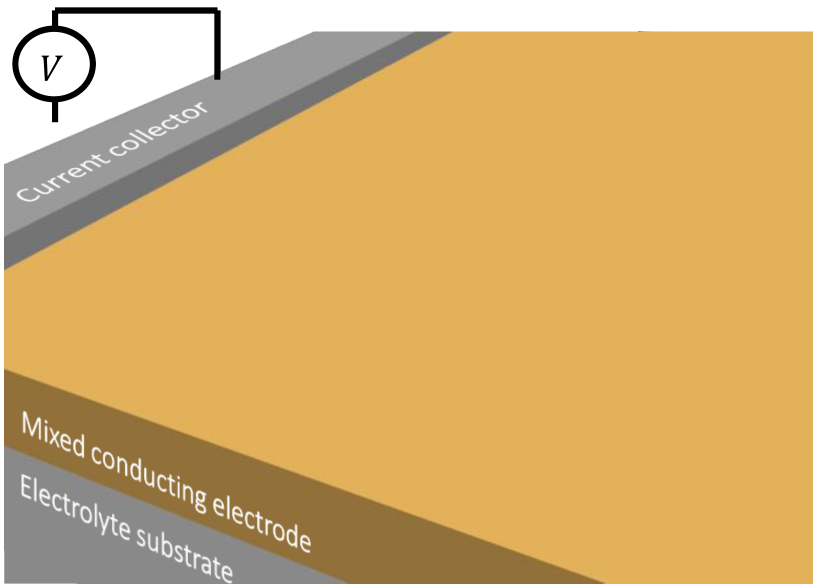
Actual Electrode with complex interfaces



Nature Nanotechnology 14 (2019) 245

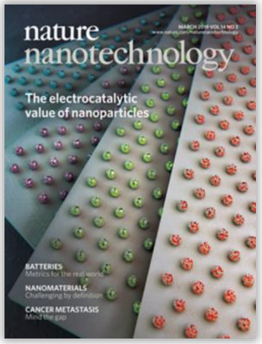
- Chemical & Morphological Complexities
- Coupled Surface & Diffusion Reactions
- Uneven Dispersion of Infiltrated Particles
- Unstable Nanoparticle Structures

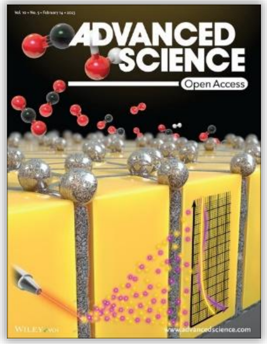
Model Electrode with well-defined interface

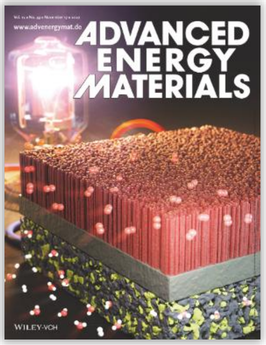


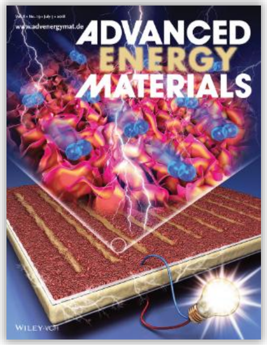
- Well-defined Thin-film Electrode Structures
- Selective Analysis of Surface Reactions
- Uniform Dispersion of Patterned Particles
- Stable & Size-controllable Nanoparticles

2. Model System Study with Well-defined Interfaces







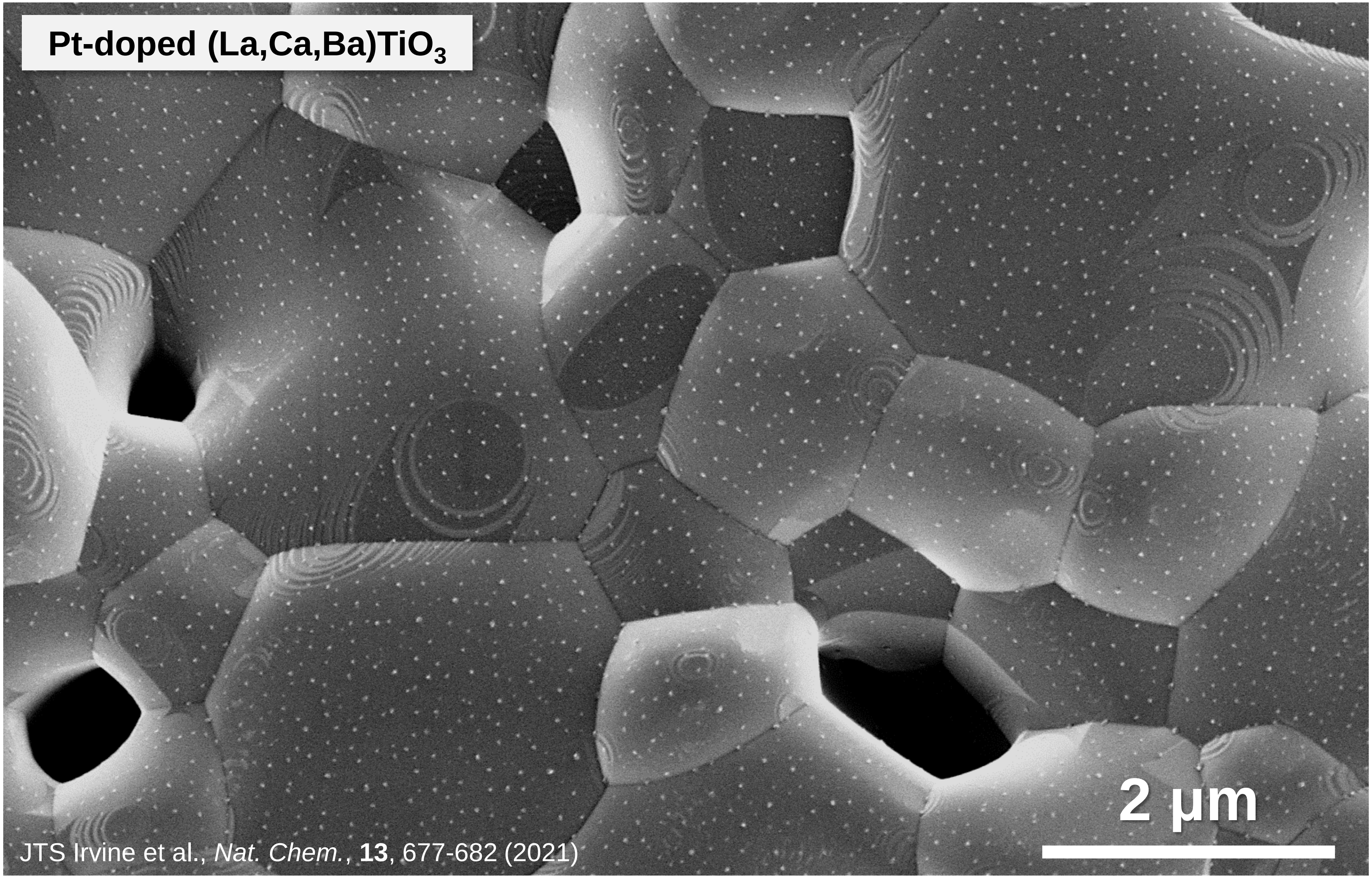


Adv. Science (2023) IF = 15.1	NPG Asia Mater. (2022) IF = 9.7	Energy Environ. Sci. (2022) IF = 32.5	Chem (2022) IF = 23.5	Energy Environ. Sci. (2020) IF = 32.5	Adv. Mater. Interfaces (2020) IF = 5.4
J. Mater. Chem. A (2020) IF = 11.9	J. Mater. Chem. A (2020) IF = 11.9	ACS AMI (2020) IF = 9.5	JACS (2019) IF = 15.0	Nature Nano-technol. (2019) IF = 38.3	Energy Environ. Sci. (2018) IF = 32.5
Nature Comm. (2018) IF = 16.6	Adv. Energy Mater. (2018) IF = 27.8	ACS AMI (2018) IF = 9.5	J. Mater. Chem. A (2018) IF = 11.9	Acta Materialia (2016) IF = 9.4	Nano Energy (2016) IF = 17.6
J. Mater. Chem. A (2016) IF = 11.9	Energy Environ. Sci. (2014) IF = 32.5	Nature Mat. (2012) IF = 47.66	Energy Environ. Sci. (2012) IF = 32.5	Energy Environ. Sci. (2012) IF = 32.5	Adv. Energy Mater. (2011) IF = 27.8

25 related articles have been published.

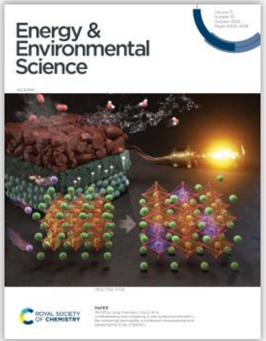
3. Cation Separation on the Complex Oxide Surface

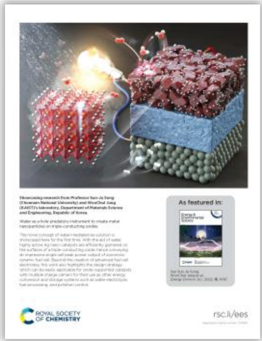
***In situ* growth of metal nanoparticles directly from an oxide support**

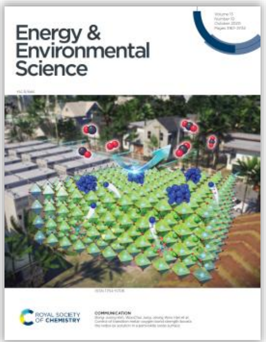


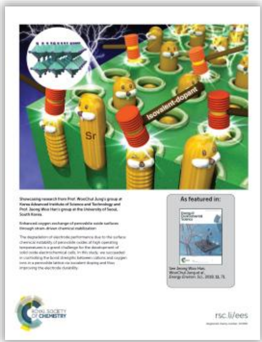
JTS Irvine et al., *Nat. Chem.*, **13**, 677-682 (2021)

Surface Phase Separation in Complex Oxides







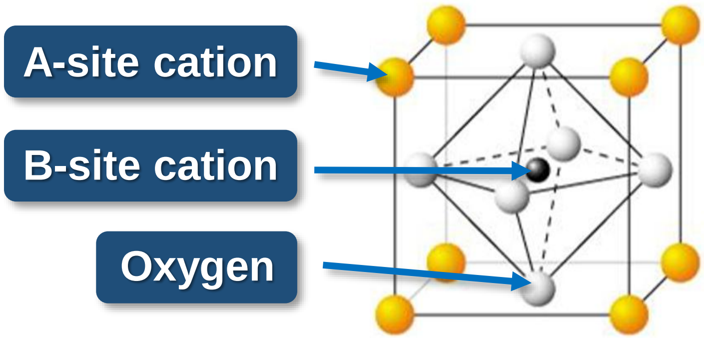


30 related articles have been published.

Appl. Catal. B: Environ. (2023) IF = 22.1	ACS Nano (2023) IF = 17.1	Advanced Science (2023) IF = 15.1	Adv. Mater. (2023) IF = 29.4	Appl. Catal. B: Environ. (2022) IF = 22.1	Energy Environ. Sci. (2022) IF = 32.5
ACS Catalysis (2022) IF = 12.9	Adv. Mater. (2022) IF = 29.4	J. Mater. Chem. A (2022) IF = 11.9	ACS Nano (2022) IF = 17.1	Energy Environ. Sci. (2021) IF = 32.5	ACS Nano (2021) IF = 17.1
Adv. Mater. (2020) IF = 29.4	Energy Environ. Sci. (2020) IF = 32.5	J. Mater. Chem. A (2020) IF = 11.9	Adv. Funct. Mater. (2020) IF = 19	ACS AMI (2020) IF = 9.5	JACS (2019) IF = 15
Nature Comm. (2018) IF = 16.6	Joule (2018) IF = 39.8	Energy Environ. Sci. (2018) IF = 32.5	Energy Environ. Sci. (2014) IF = 32.5	Energy Environ. Sci. (2012) IF = 32.5	Energy Environ. Sci. (2012) IF = 32.5

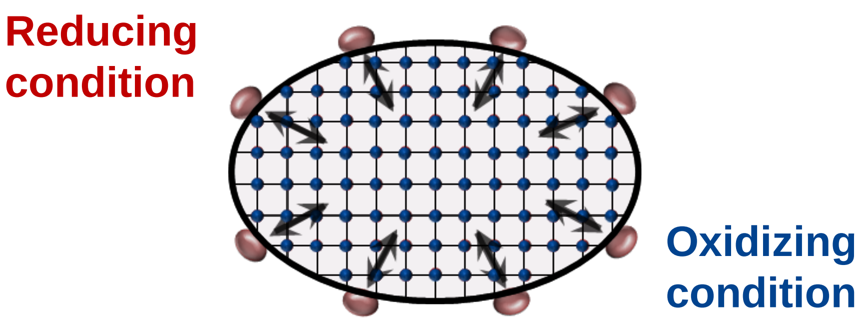
Ex-solution Phenomenon

Selective reduction of transition metal cations in a complex oxide

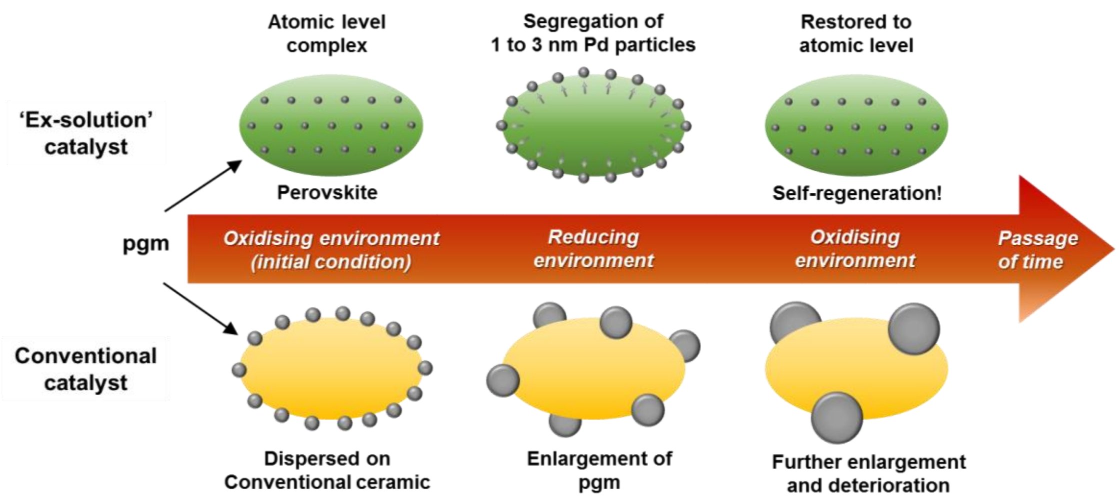


Perovskite structure (ABO_3)

B-site: transition or precious metals



$$ABO_3 \leftrightarrow AB_{1-x}O_{3-\delta} + xB + \frac{\delta}{2}O_{2(g)}$$



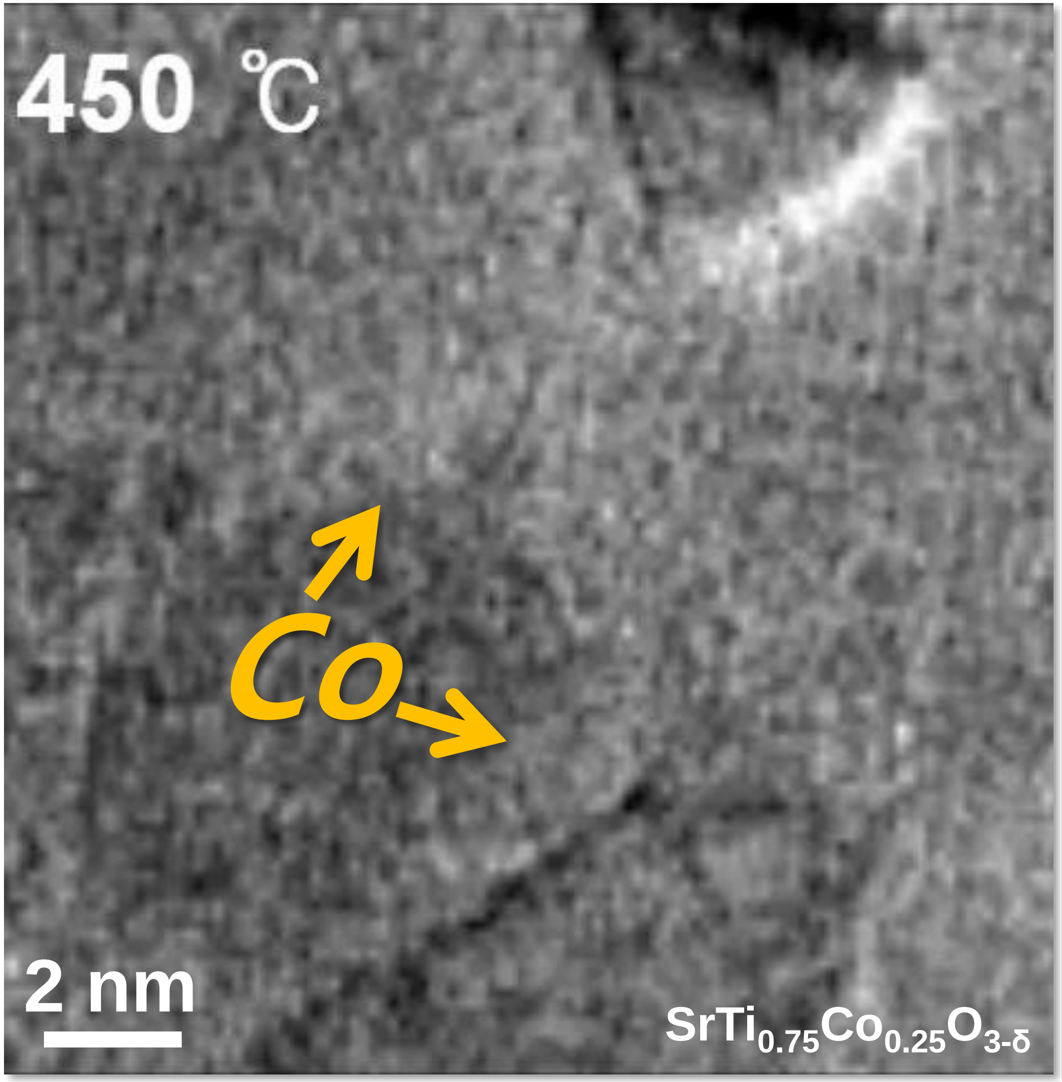
Advantages

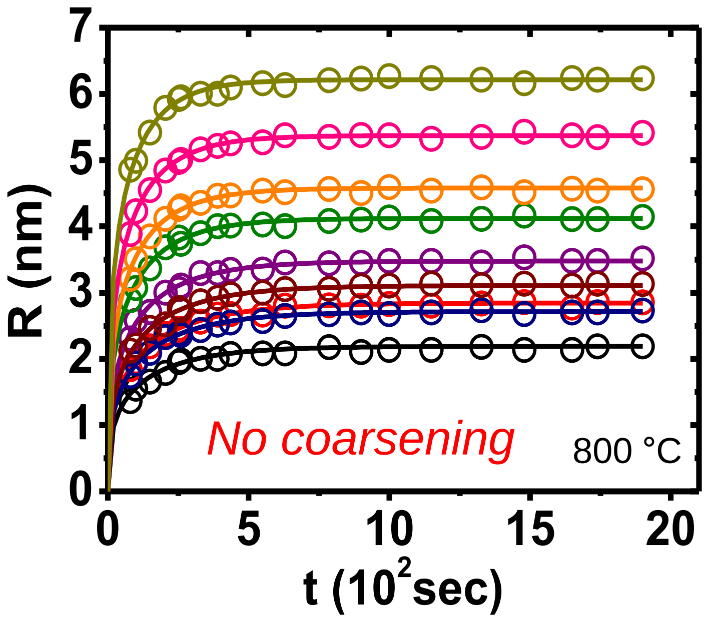
- Fast & cost-effective synthesis
- Fine & uniform particle dispersion
- Reversibility → long life time
- Strong anchorage to support

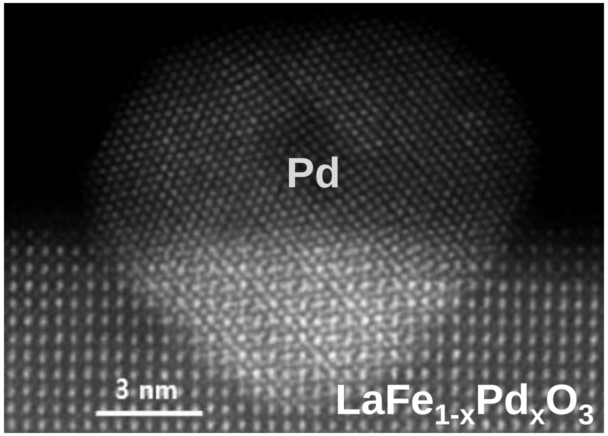
Strong Binding to Host Lattice

In courtesy of B. -J. Kim

High durability of ex-solved nanoparticles: Thermal Stability





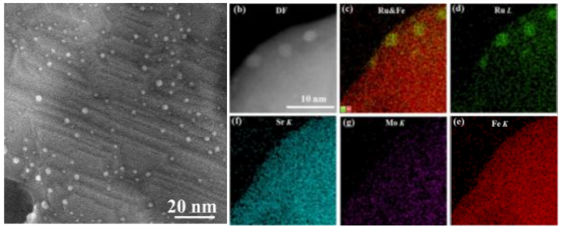


W. Jung et al., *J. Am. Chem. Soc.* **141**, 6690−6697 (2019)

J. Am. Chem. Soc., **133**, 18506 (2011)

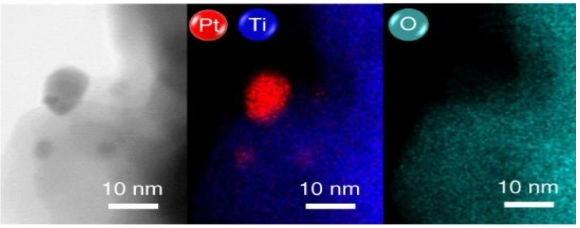
Related Research Status

Ru-Fe in Sr(Fe,Ru,Mo)O_3



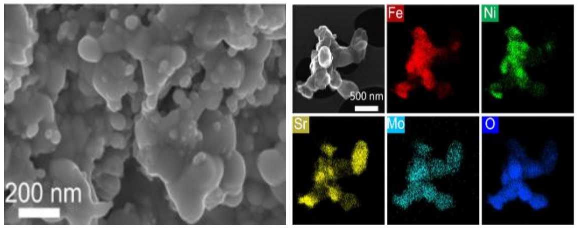
Nat. Commun., **12**, 5665 (2021)

Pt in (La,Ca/Sr,Ba)(Pt,Ti)O_3



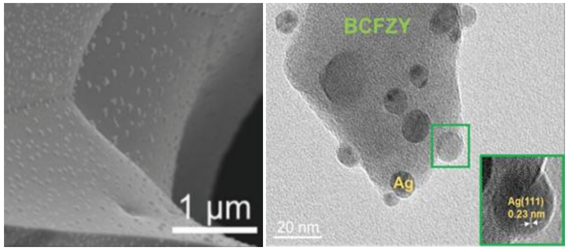
Nat. Chem., **13**, 677 (2021)

Ni-Fe in Sr_2(Fe,Ni,Mo)O_6



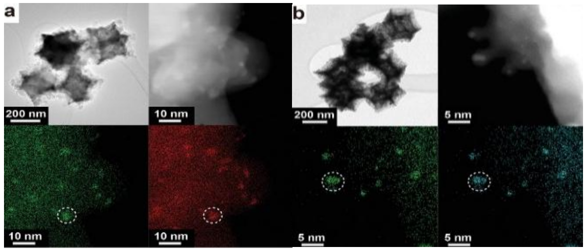
Nat. Commun., **13**, 4618 (2022)

Ag in Ba(Co,Fe,Zr,Y)O_3



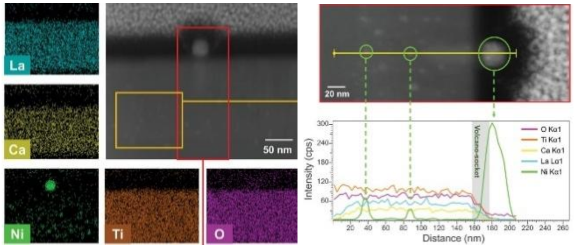
Energy Environ. Sci., **15**, 1097 (2022)

Pd-Pt/Rh in ZnO MOF



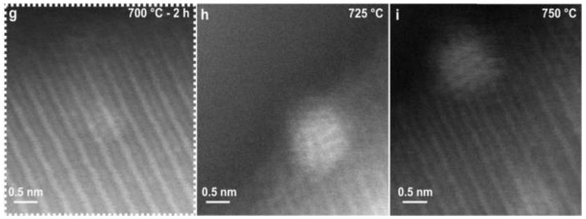
Adv. Mater., **34**, 2201109 (2022)

Ni in (La,Ca)(Ni,Ti)O3



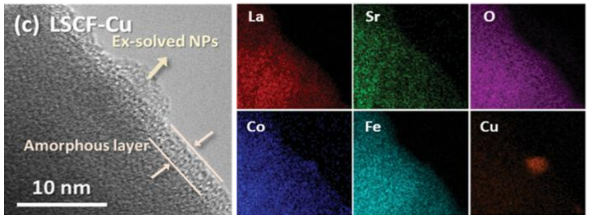
Adv. Mater., **35**, 2208984 (2023)

Ir in SrTiO3



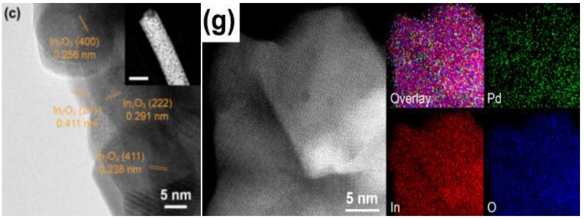
Nat. Commun., **14**, 1754 (2023)

Cu in (La,Sr)(Co,Fe)O_3



Adv. Mater., **36**, 2404103 (2024)

Pd in In_2O_3



ACS Nano, **18**, 25577 (2024)

Our Ex-solution Studies

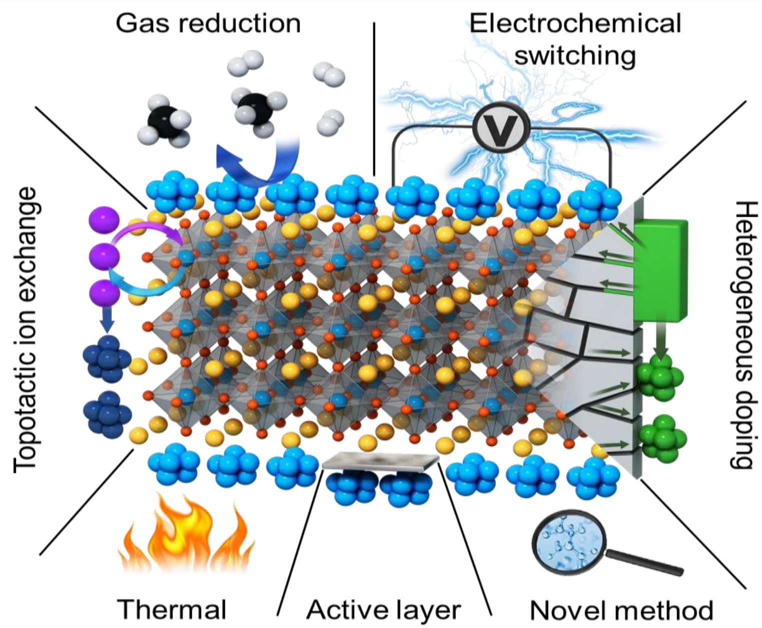
Detailed research strategies

1. Ex-solution energetics
(Ex-solution driving force)

2. Ex-solution dynamics
(Particle formation mechanism)

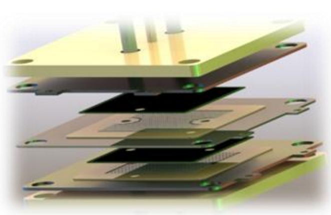
3. Advanced ex-solution process
(New synthetic routes)

Novel approaches for ex-solution



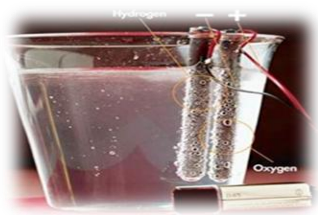
W. Jung et al., ACS Nano ***15****, 81-110 (2021)*

Use of this concept to various applications



HT-ceramic devices

Gas reformers



LT electrochemical devices

Gas sensors

Chemical looping

Summary

- Hydrogen energy technology is crucial for achieving Net Zero by 2050.
- The performance of devices for hydrogen production, storage, and utilization relies on catalyst development.
- Emerging strategies to overcome supported catalyst limitations, along with Korea-Germany collaboration, offer new possibilities.

Acknowledgement

Sustainable Energy Materials Laboratory (SEML)

Thank you for your attention

2025 Energy Transition
The 8th KAST-Leopoldina Bilateral Symposium Perspectives on Energy Transition

Atomically Dispersed Electrocatalysts for Water Electrolysis and Fuel Cell

Jinwoo Lee

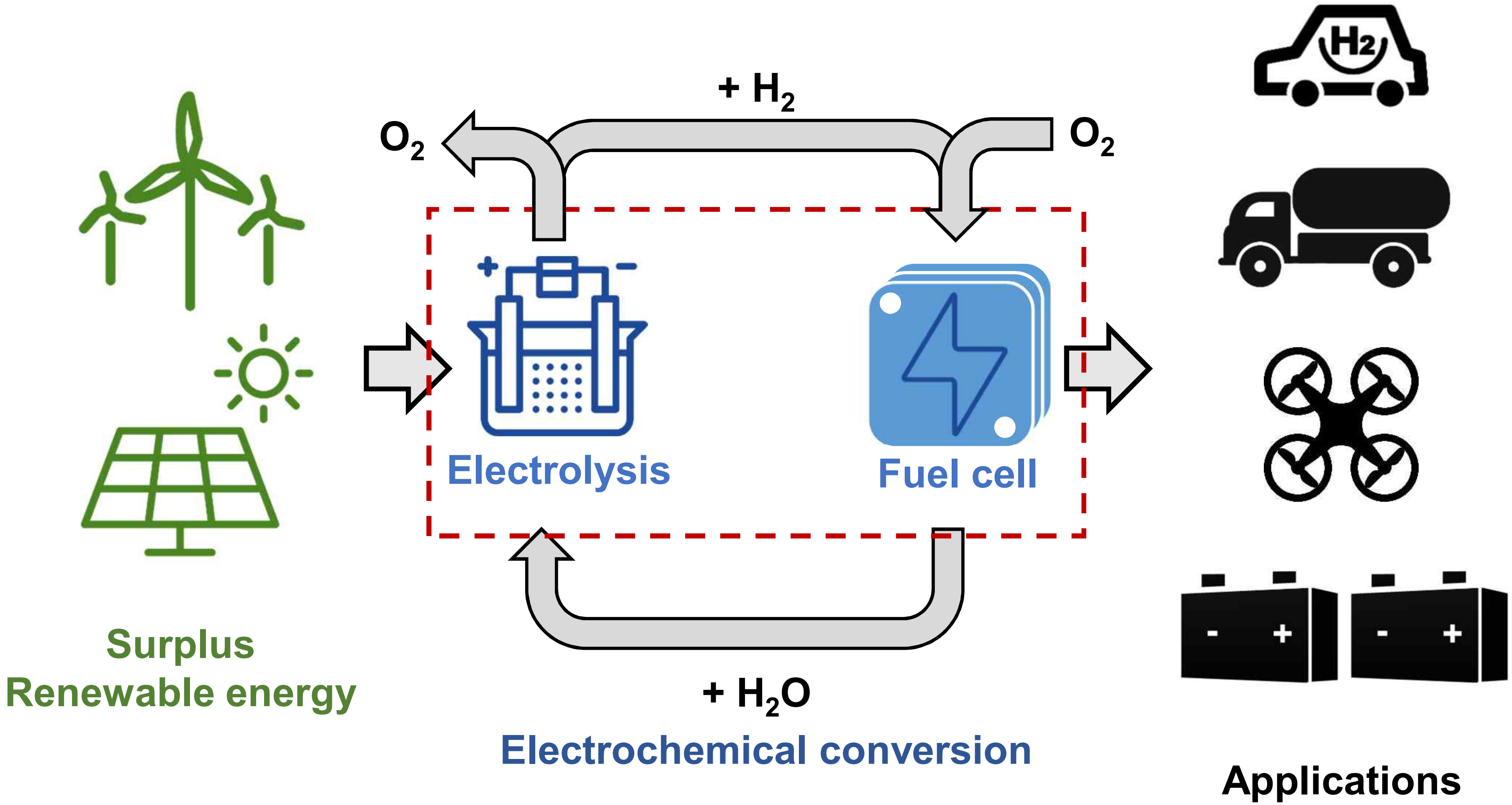
Department of Chemical & Biomolecular Engineering

KAIST

Jan. 14th, 2025

Requirement of CO_2 emission reduction technology

» High energy density & Zero emission of CO_2 in **Hydrogen cycle**



› **Electrochemical conversion devices are key component**

Hydrogen Technology in Korea
:One of National 12 Strategic Technology

1. Hydrogen Production via Water Electrolysis
2. Hydrogen Storage & Tranportation
3. Hydrogen Fuel Cells and Power Generaion

National Hydrogen Key Laboratories

(Ministry of Science and Technology, Launched in 2024: 5 year project)

Center for PEMWE

KIST 한국과학기술연구원 Korea Institute of Science and Technology

Center for AWE

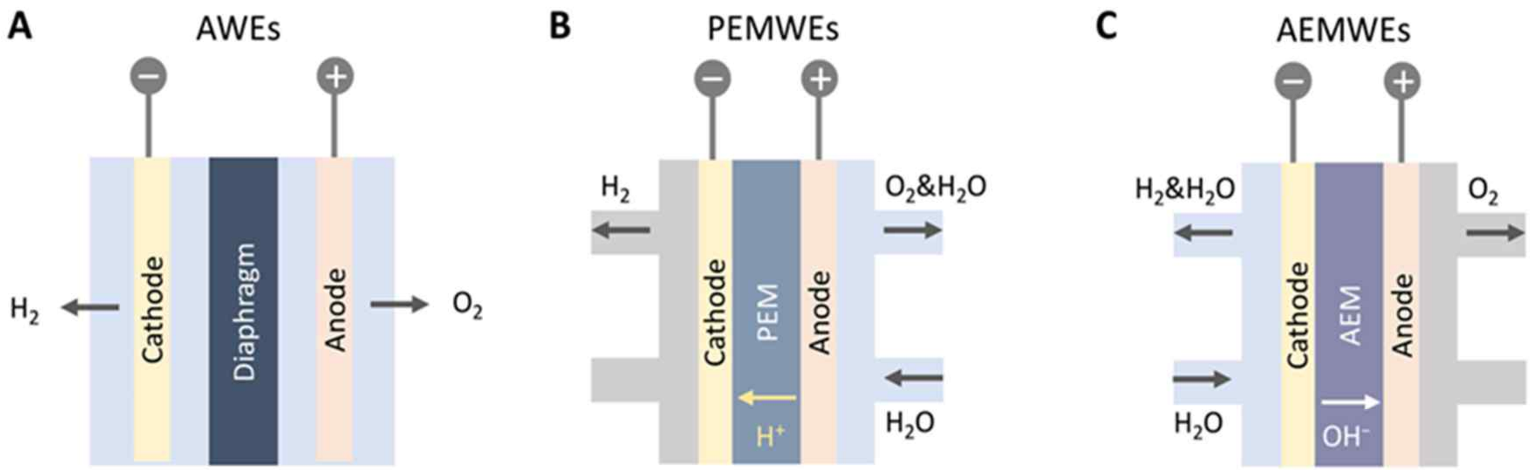
KIER 한국에너지기술연구원 KOREA INSTITUTE OF ENERGY RESEARCH

Center for AEMWE

KIMS 한국재료연구원 Korea Institute of Materials Science

Centers Collaborate with LG Chem, Samsung Engineering. Hyundai Motors…

Advantageous and Challenges in Low Temperature WE system



A – AWEs

Pros
- Non-noble catalysts
- Long-term stability

Cons
- High ohmic loss
- Low current density
- High gas sensitivity

B – PEMWEs

Pros
- Low ohmic loss
- High current density

Cons
- Acidic corrosive environment
- **Noble catalysts (IrO_x)**
- High cost of components

C – AEMWEs

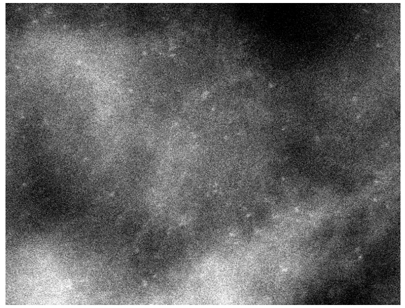
Pros
- Non-noble anode catalysts
- Low ohmic loss

Cons
- Cathode sluggish kinetics
- **Noble cathode catalysts**
- **Issues on membranes**

Sci .Adv. **2023**, 9, eadi7755

Atomically Dispersed Electrocatalysts

Atomically dispersed catalysts (ADCs);
Individual, isolated atoms deposited on a desired support

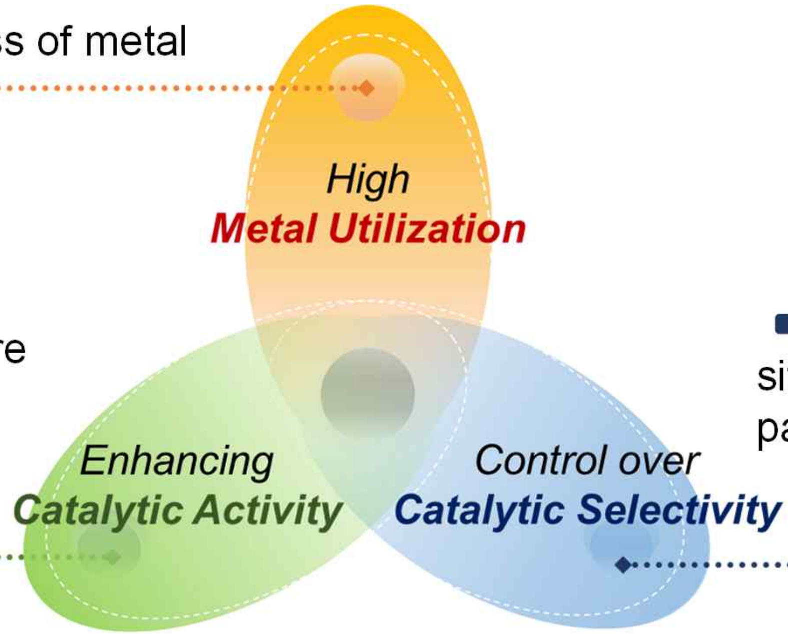


“Pt SAC/S-doped C”

» ADCs composed of 1) metals and 2) supports

1) Supported metals

- Minimization of metal
- High activity per unit mass of metal



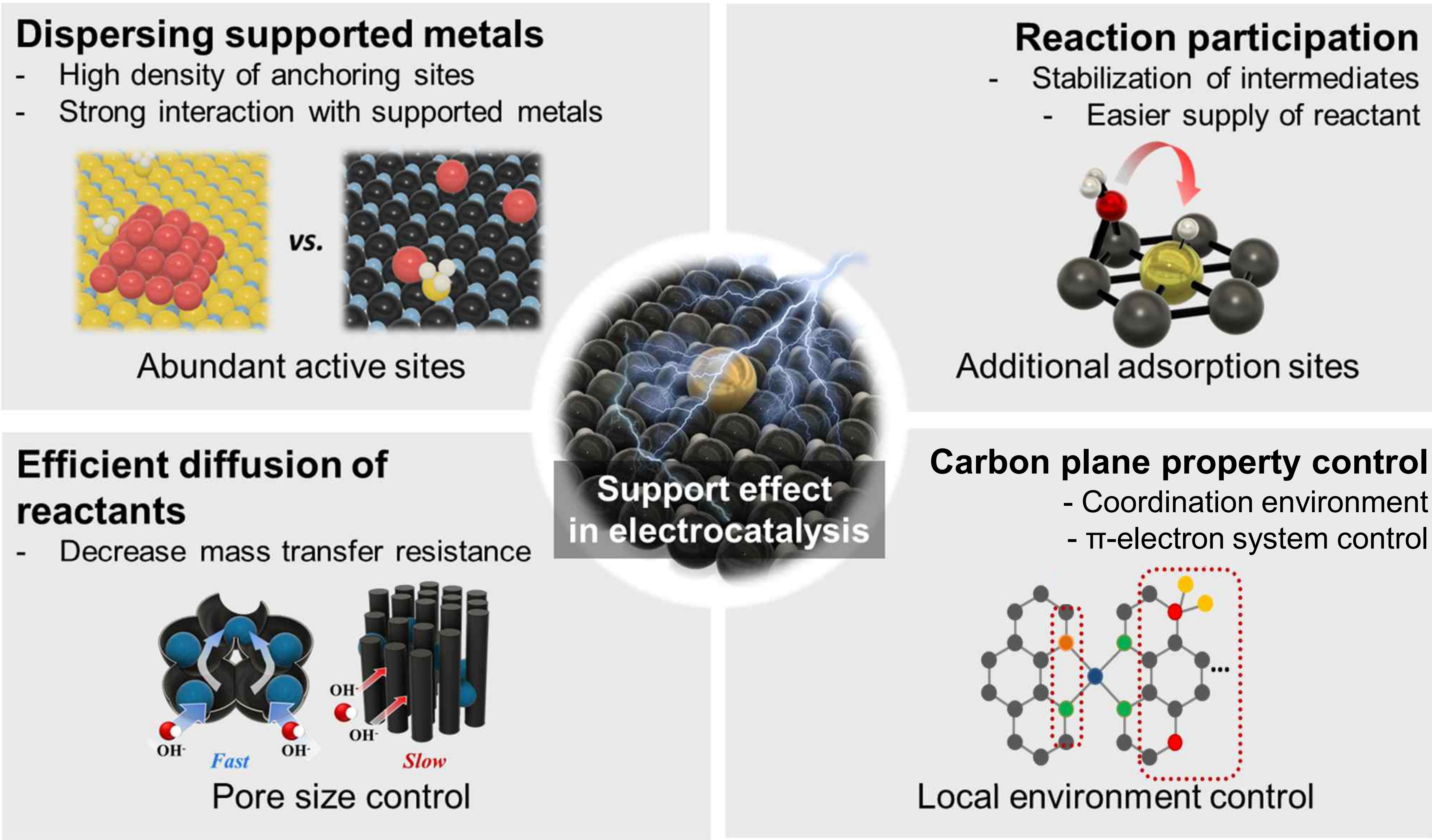
- Tuning electronic structure *via* supported metal species

- Absence of metal ensembl sites can change the reaction pathway.

✓ ***Completely different catalytic properties*** can be observed on ADCs, compared to nano- and bulk-catalysts.

Atomically Dispersed Electrocatalysts

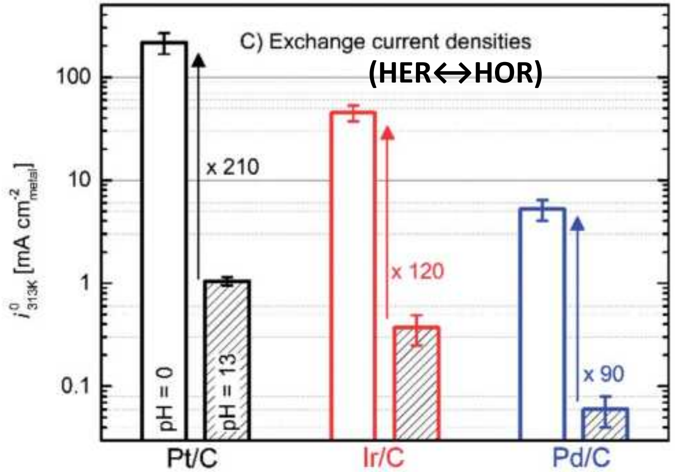
2) Support materials effects



✓ ***Thorough understanding of the function of the supports*** *is required in designing effective ADCs with superior activity and stability.*

Challenges of Alkaline Hydrogen Electrocatalysts

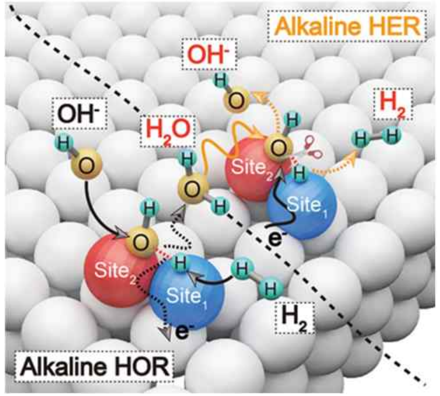
» Sluggish kinetics in alkaline condition



Energy Environ. Sci. **2014**, 7, 2255-2260

Acidic electrolyte	
$2H_{(aq)}^{+} + 2e^{-} \rightarrow H_{2(g)}$	
Volmer step	$H^{+} + e^{-} \rightarrow H_{ads}$
Tafel step	$2H_{ads} \rightarrow H_2$
Heyrovsky step	$H^{+} + H_{ads} + e^{-} \rightarrow H_2$
Alkaline electrolyte	
$2H_2O + 2e^{-} \rightarrow H_{2(g)} + 2OH_{(aq)}^{-}$	
Volmer step–water dissociation	$2H_2O + 2e^{-} \rightarrow 2H_{ads} + 2OH^{-}$
Tafel step	$2H_{ads} \rightarrow H_2$
Heyrovsky step	$H_2O + H_{ads} + e^{-} \rightarrow H_2 + OH^{-}$

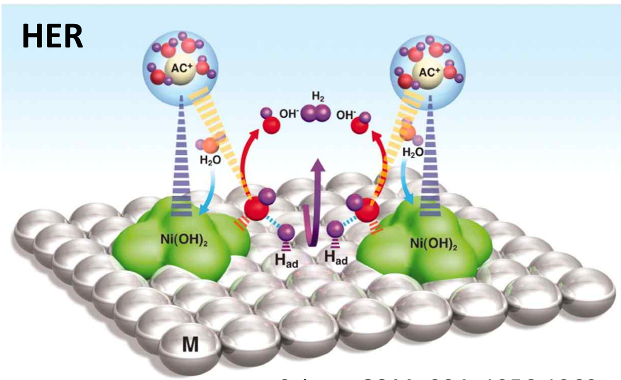
Mechanism of hydrogen evolution reactions in acidic and alkaline solution



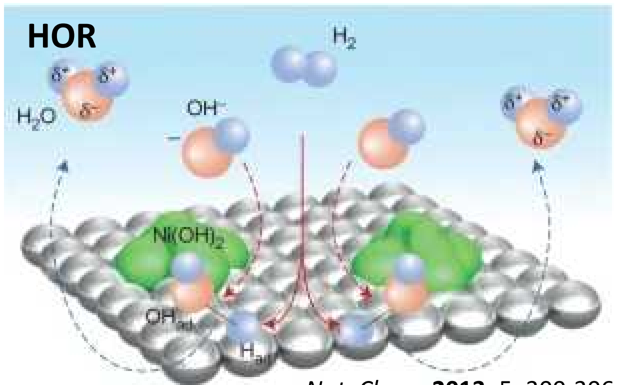
Adv. Funct. Mater. **2022**, 32, 2107479

Alkaline → 2 order of magnitude sluggish kinetics than acidic ➔ additional OH* site required

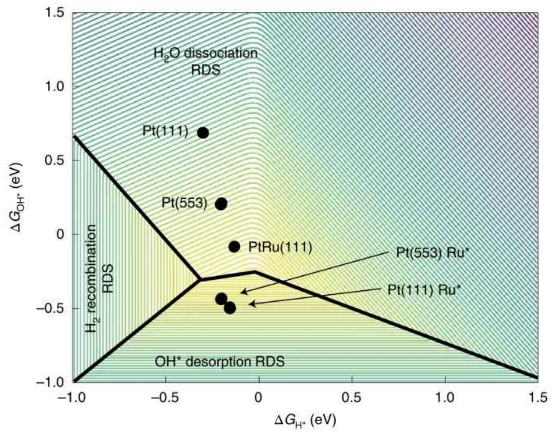
» Strategies to overcome sluggish alkaline HER kinetics



Science **2011**, 334, 1256-1260



Nat. Chem. **2013**, 5, 300-306



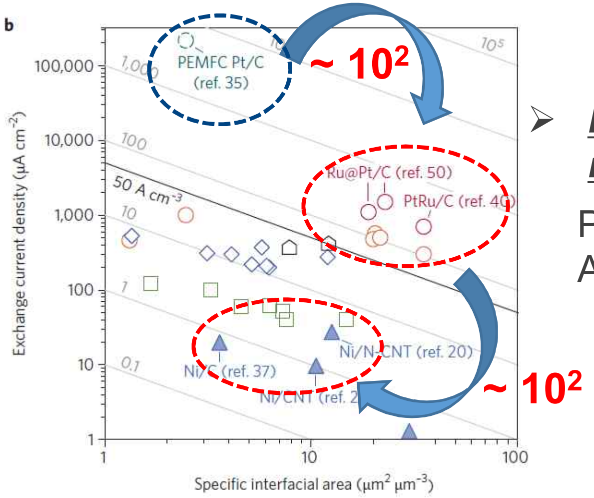
Nat. Energy **2020**, 5, 891-899

➔ Oxophilic hydroxide ($Ni(OH)_2$) & 2nd metals (Ru, Ir) used to overcome the sluggish kinetics

Rational Design of Supports for Alkaline HOR

Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

Sluggish kinetics in alkaline condition

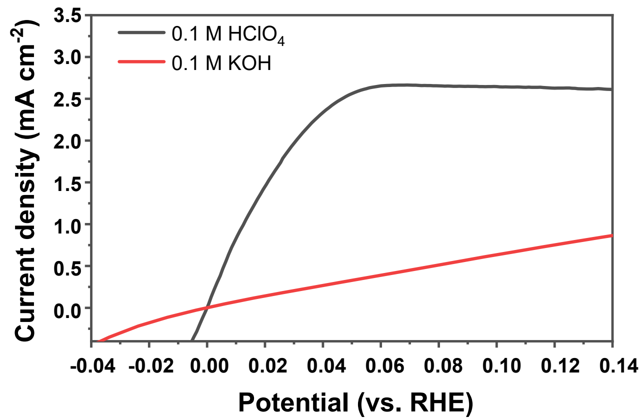


➢ ***Higher Pt loading in anode is needed***

PEMFCs (0.05 mg_{Pt} cm^{-2})
AEMFCs (0.4 mg_{Pt} cm^{-2})

Energy. Environ. Sci., 2014, 7, 2255
Nat. Nanotech., 2016, 11, 1020

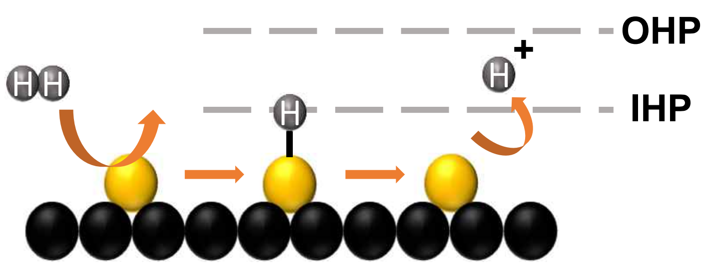
➢ ***0.8 wt% Pt SA/S-doped carbon***



The difference is incorporation of OH^-.

Understanding alkaline HOR in SACs

- HOR in acidic condition

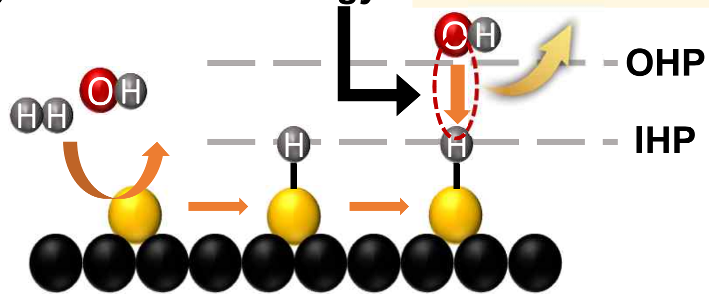


Single-atom on carbon

- HOR in alkaline condition

Higher activation energy

Non-covalent interaction becomes important.



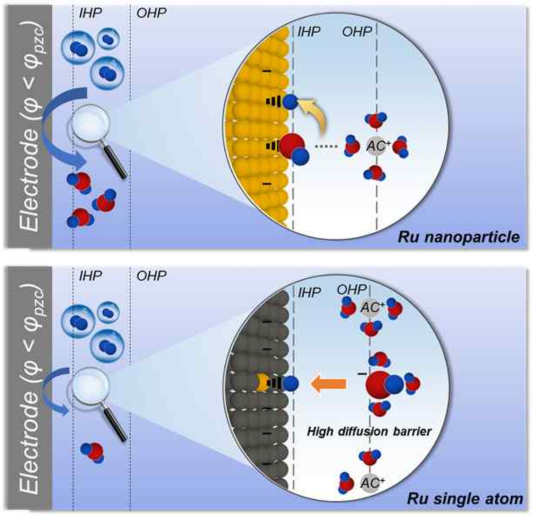
Single-atom on carbon

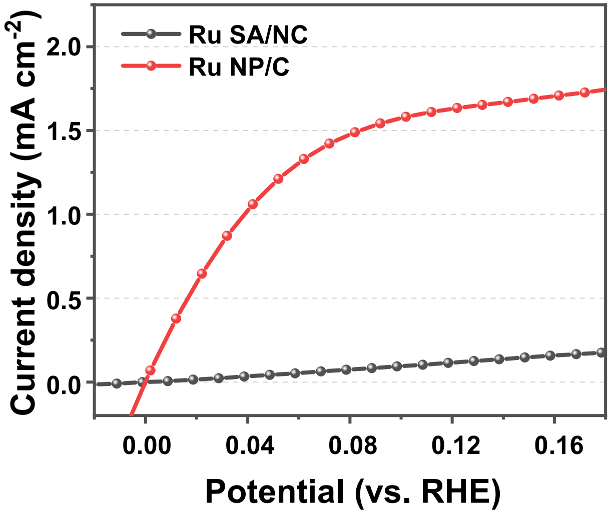
Activity: Dependent on **HBE** | **HBE** & **Non-covalent interaction**

Rational Design of Supports for Alkaline HOR

Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

Carbon-supported Ru SACs for HOR



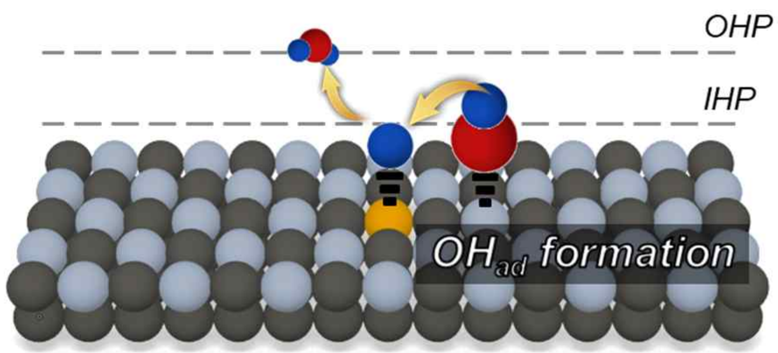


<Electrochemical half-cell test condition>

- Electrolyte: H_2-saturated 1M KOH
- Chronopotentiometry: Currents was obtained after holding 30 s at interval of 10 mV with 1600 rpm
- Reference: Hg/HgO, Counter electrode: carbon rod
- Ru loading: 4 ug on GC

Significantly reduced HOR activity of SACs compared to NPs

Rational design of support materials in SACs for HOR



Schematic illustration of HOR mechanism

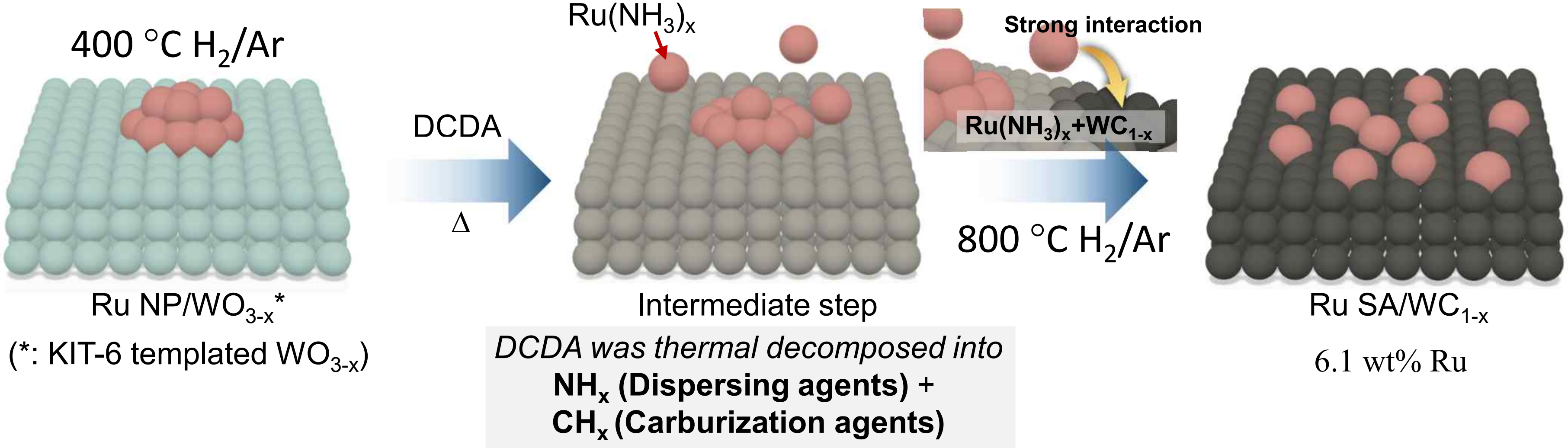
Requirement in support materials

- ***Capable of providing of OH group***
- ***Strong interaction with noble metal to synthesize SACs at high temperature***
- ***High electron conductivity***

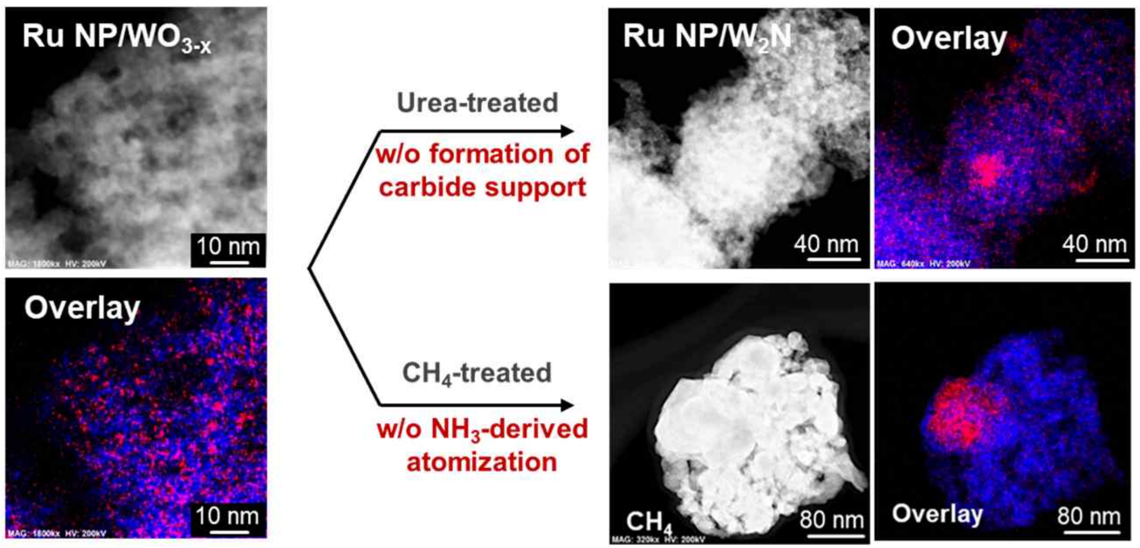
Rational Design of Supports for Alkaline HOR

Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

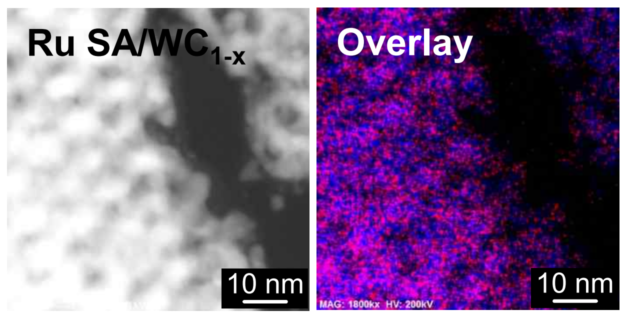
Synthesis process of tungsten carbide (WC_{1-x})-supported Ru SACs



EDX-mapping results



DCDA-treated sample

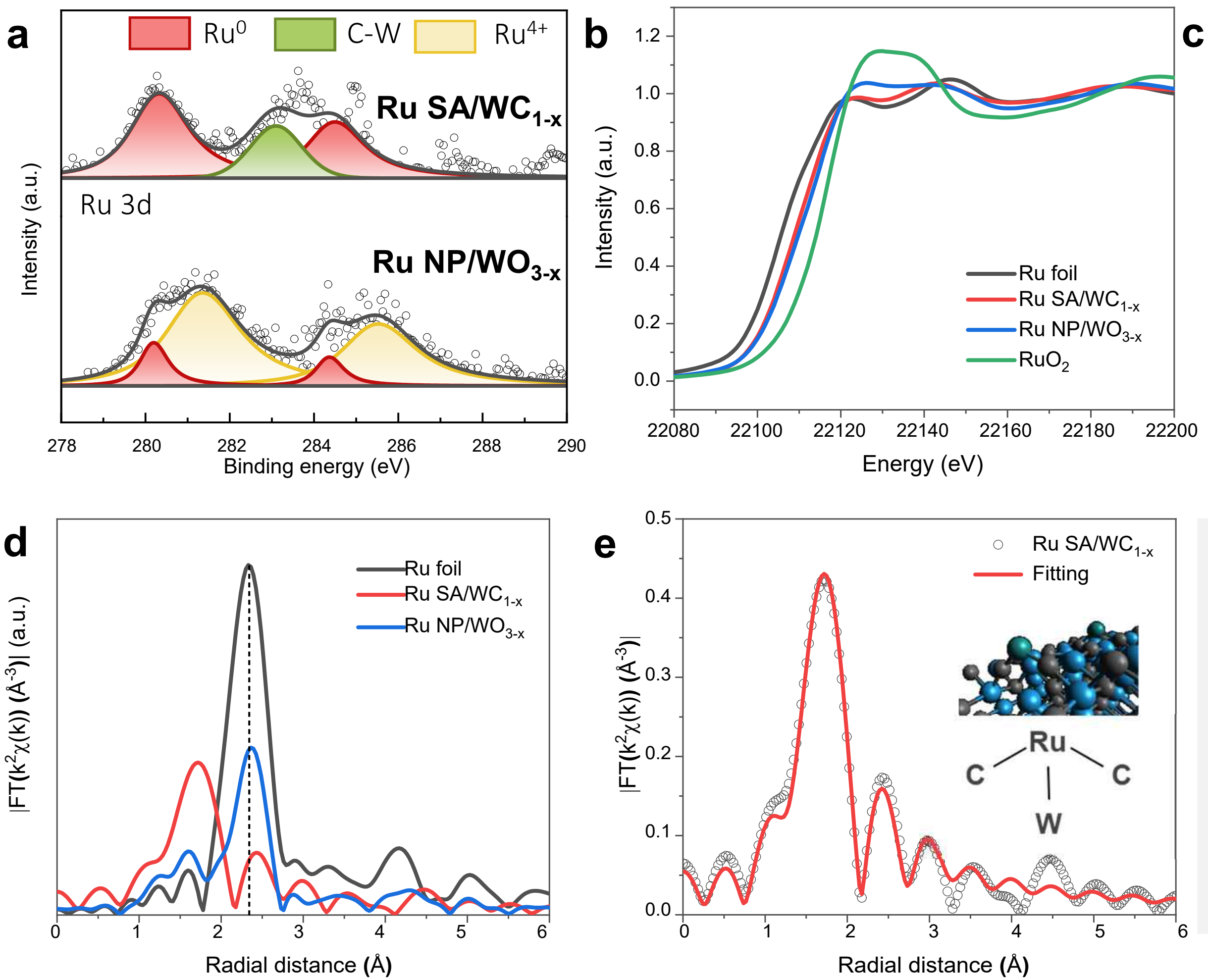


Highly dispersed Ru atoms

Rational Design of Supports for Alkaline HOR

Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

XPS & XAS characterization

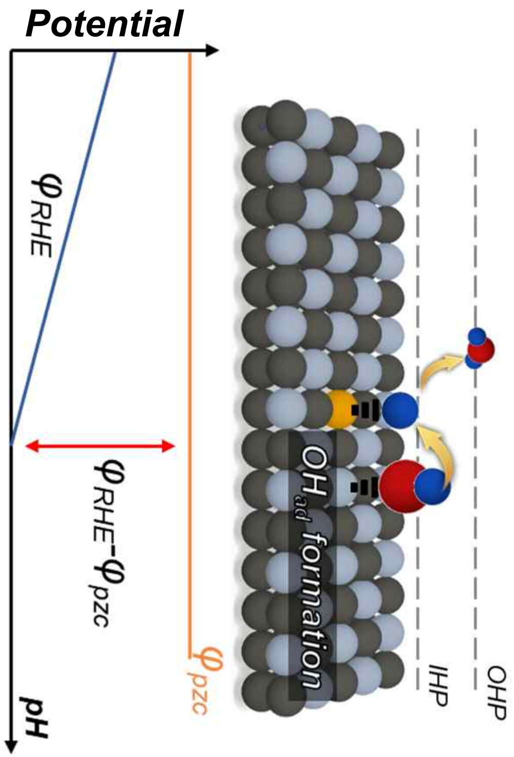


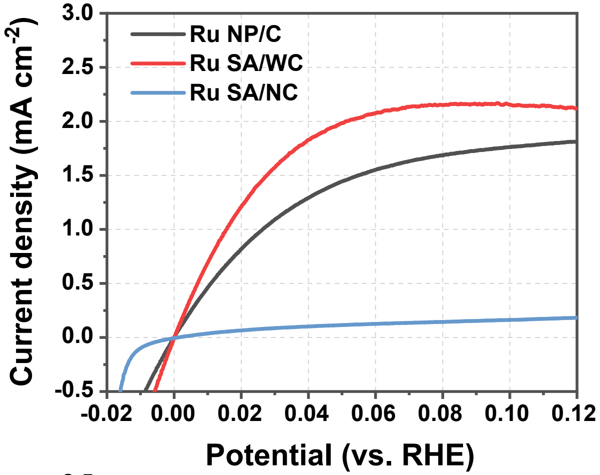
- ✓ Ru SA/WC_{1-x} showed metallic property, suggesting strong interaction with metallic WC_{1-x} support.
- ✓ **Ru SA/WC_{1-x} was composed of Ru-C path and Ru-W path**

Rational Design of Supports for Alkaline HOR

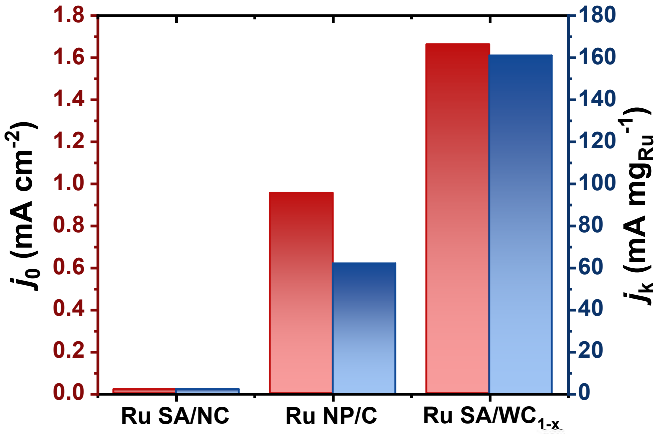
Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

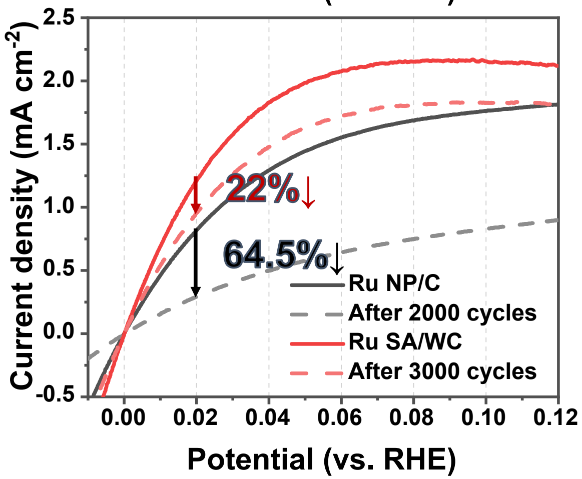
» Electrochemical characterization

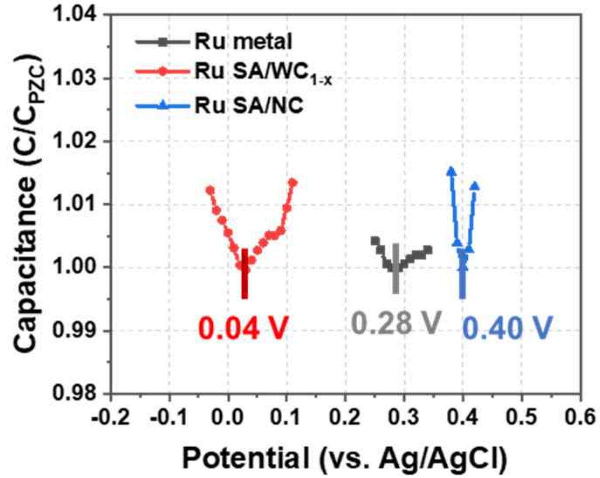




@20 mV







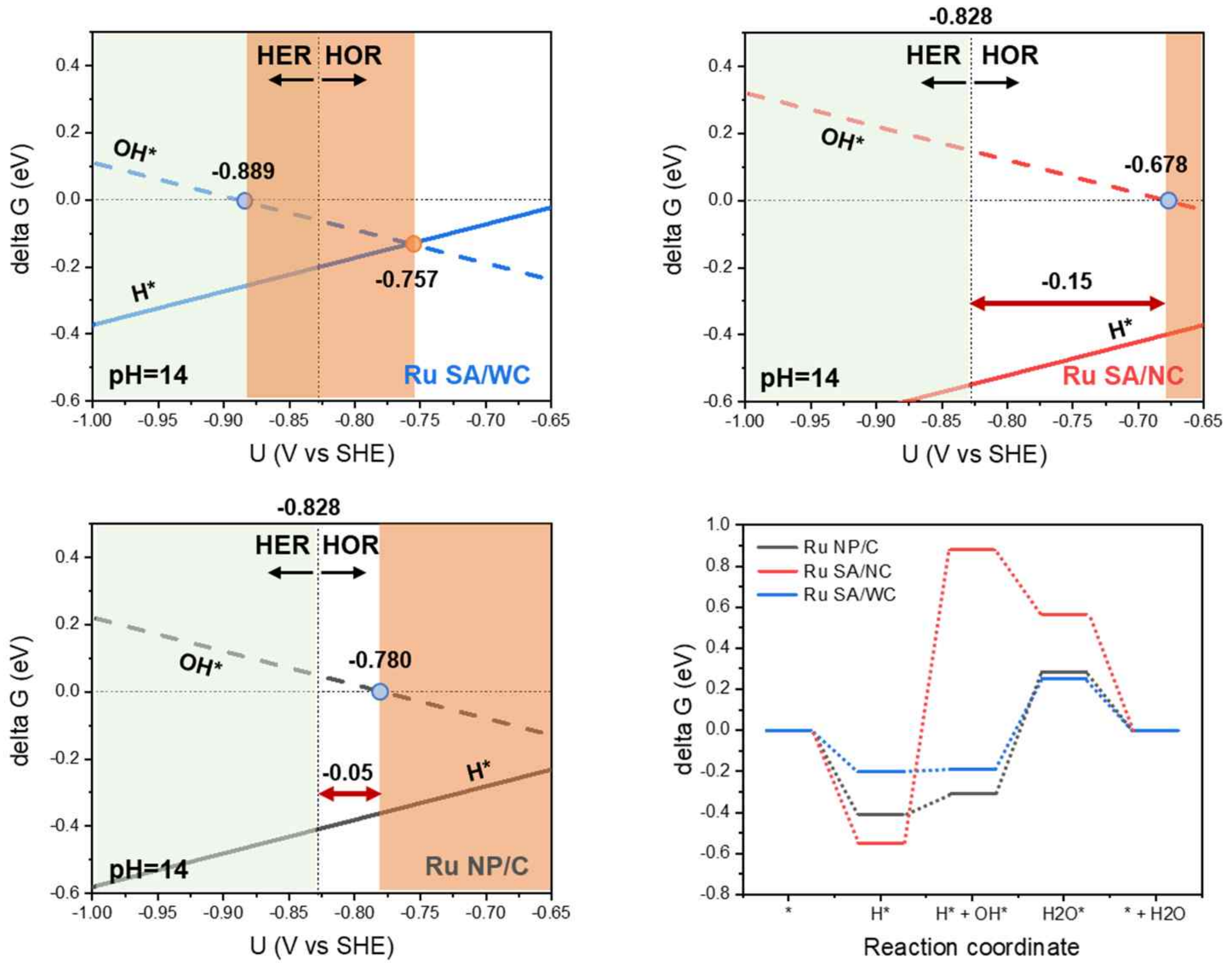
- ✓ Ru SA/NC showed negligible catalytic activity for HOR, whereas Ru SA/WC_{1-x} exhibited outstanding activity of 1.22 mA cm^{-2}. Also, Ru SA/WC_{1-x} showed 2.6 times higher mass activity (j_M @ 20mV) than that of Ru NP/C.
- ✓ It was confirmed that potential of zero charge (PZC) decreased in the order of Ru SA/NC, Ru metal, Ru SA/WC_{1-x}, which means that diffusion of OH^- into the electrode was facilitated by WC_{1-x}.

Rational Design of Supports for Alkaline HOR

Jinwoo Lee et al, Adv. Mater.* **2024**, 36, 2308899

» DFT calculation

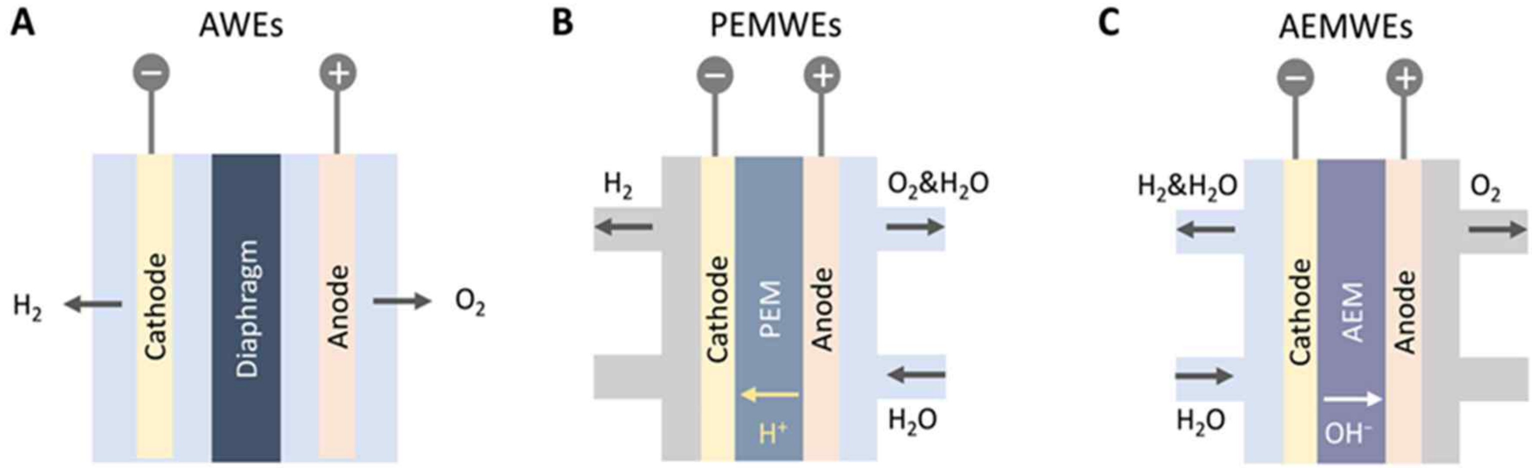
Prof. Jihan Kim
(KAIST)



- ✓ Ru SA/NC need high overpotential of 0.15 V to accommodate OH, but Ru SA/WC_{1-x} showed high affinity for OH^-
- ✓ Also, the hydrogen binding energy (HBE) was optimized by the strong interaction btw Ru and WC_{1-x}.

Advantageous and Problems of AEMWE

Pros and Cons of AEMWE System



Pros
- Non-noble catalysts
- Long-term stability

Cons
- High ohmic loss
- Low current density
- High gas sensitivity

Pros
- Low ohmic loss
- High current density

Cons
- Acidic corrosive environment
- **Noble catalysts (IrO_x)**
- High cost of components

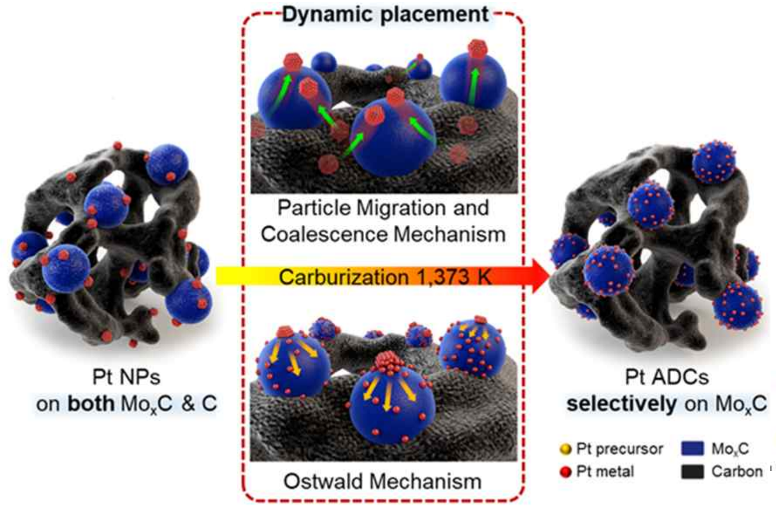
Pros
- Non-noble anode catalysts
- Low ohmic loss

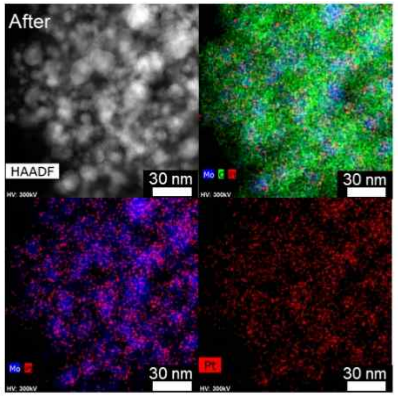
Cons
- Cathode sluggish kinetics
- **Noble cathode catalysts**
- **Issues on membranes**

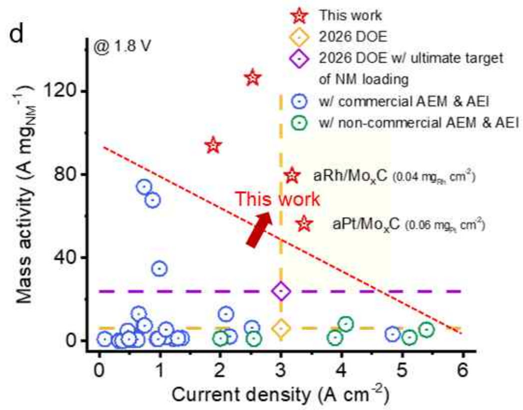
Sci .Adv. **2023**, 9, eadi7755

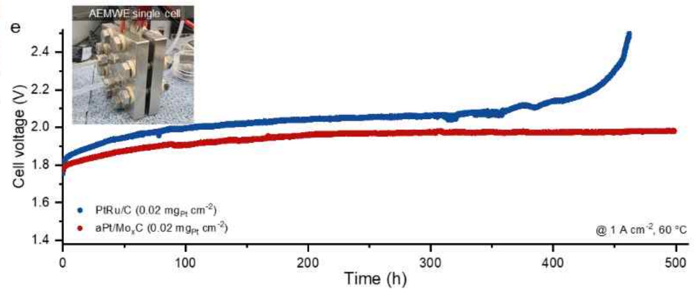
✓ Non-noble metal-based anode catalysts without corrosion → possibility to replace PEMWE system
✓ Still cathode sluggish kinetics (Hydrogen evolution reaction) → Need to reduce usage of noble metal
✓ Atomically dispersed catalysts (single atom & cluster) are suggested for AEMWE cathode electrocatalysts

Self-Assembly-Assisted Dynamic Placement of Noble Metals Selectively on Multifunctional Carbide Supports for Alkaline Hydrogen Electrocatalysis









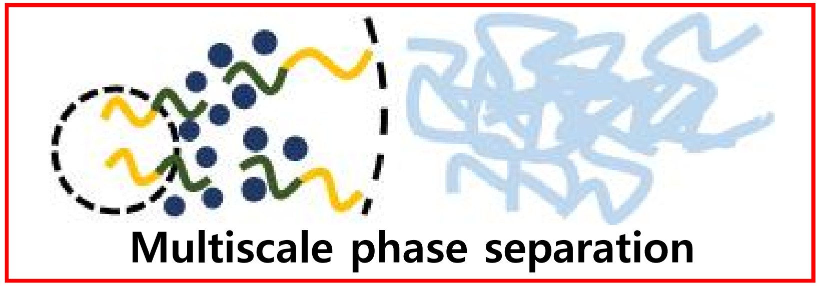
Key concepts

1. Novel synthesis (Molecular Interaction & Metal-Support Interaction)
   Spontaneous and selective placement of NM ADCs on Mo_xC
2. Multifunctional Mo_xC support
   Embody dynamic placement & Control interfacial water structure
3. Efficient AEMWE electrocatalysts
   Fulfill PEMWE 2026 DOE target with ultralow NM ($0.06\ mg_{Pt}\ cm^{-2}$)

Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

Porous Material Design for Energy

- Multiscale Self-Assembly and Nanocatalysts to synthesize various functional materials

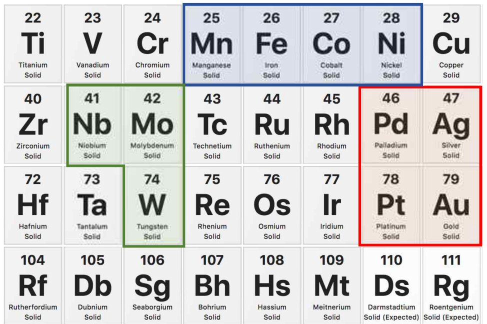


- Control of nanostructure
- Simple synthetic route
- Sol-gel chemistry
- Diversify particle properties

Acc. Chem. Res. 2023, 56, 3428.

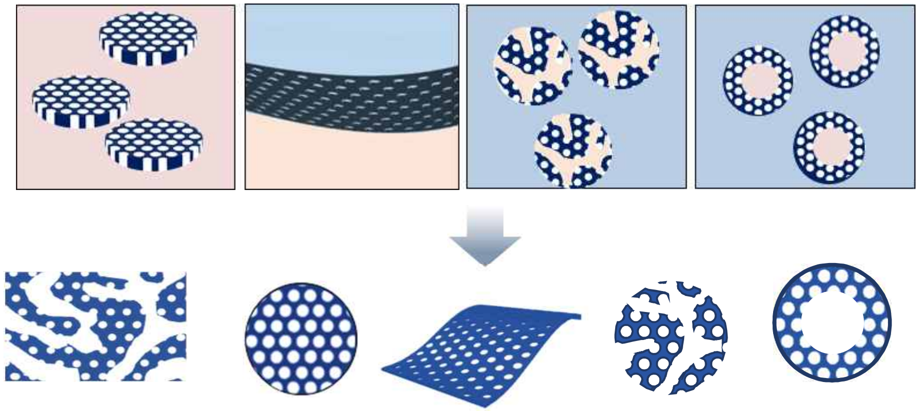
Various composition

- Metallic porous structure
- Transition metal oxdies, carbides



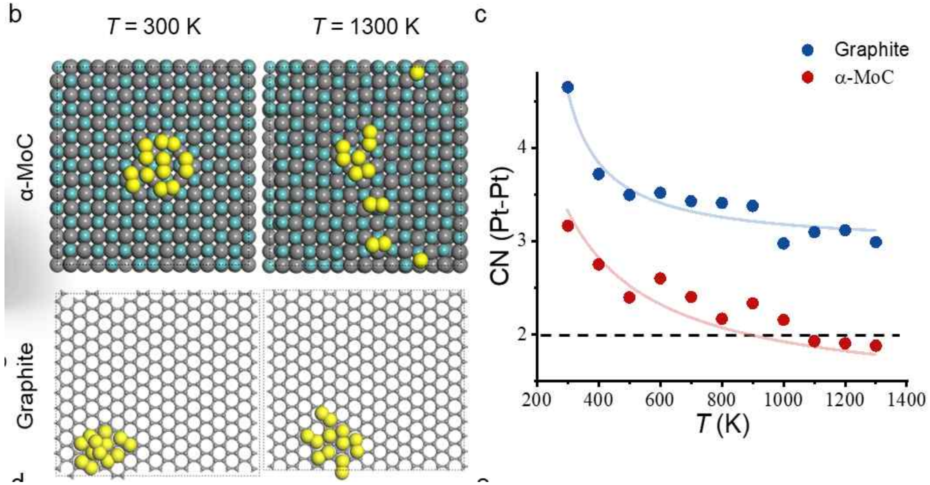
Nat. Comm. 2023, 14, 7210
Adv. Mater. 2018, 30, *1703829*
Sci. Adv. 2020, 6, *eabb3814*
J. Am. Chem. Soc. 2020, 142, *9250*
Nat. Catal. 2020, 3, *639*
Energy. Environ. Sci. 2022, 15, *3449*
Adv Mater. 2023, 35, 2208999

Structure control



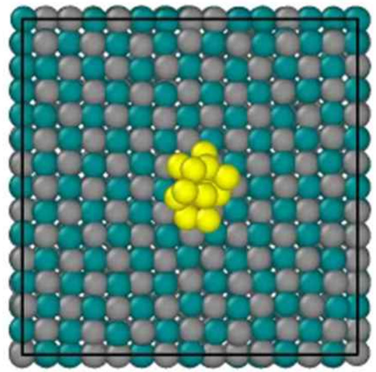
J. Am. Chem. Soc. 2014, 136, *16066*
Adv. Mater. 2019, 31, *1806547*
Adv. Mater. 2018, 30, *1707557*
Adv. Mater. 2018, 30, *1801127*
J. Am. Chem. Soc. 2021, 143, *15644*
Acc. Chem. Res. 2023, 56, 3428
Adv. Mater. 2024, 36, *2308899*
Adv Mater. *adma/202306602*

Synthesis strategy: Dynamic Placement (MSI)

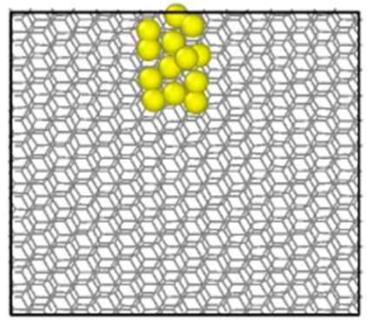


At high *T*

Pt cluster on Mo_xC

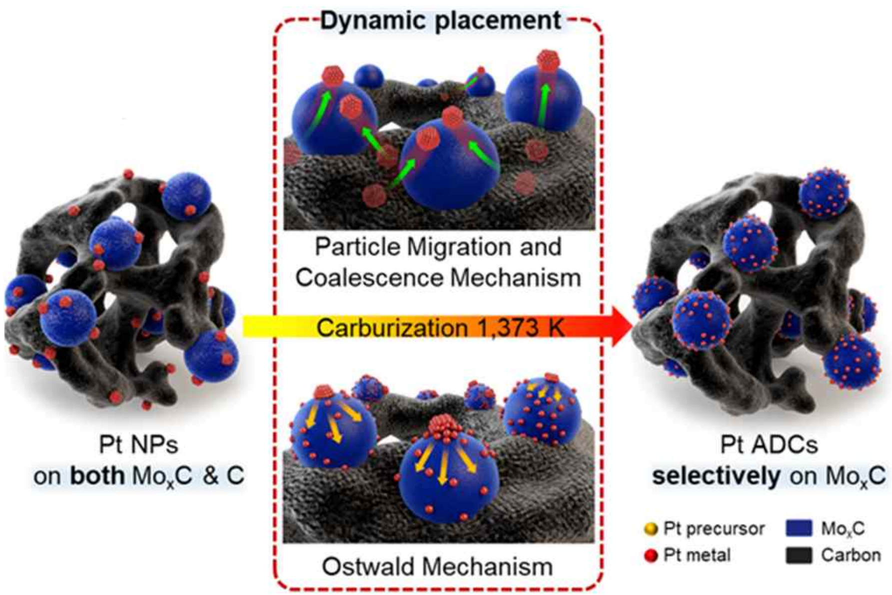


Pt cluster on Graphite



Metal-Support Interaction (MSI)

- Strong MSI (Mo_xC):
  Ostwald mechanism
- Weak MSI (Carbon):
  Particle migration and coalescence



Designing of dynamic placement at high T using different MSI

→ Spontaneous disintegration of Pt NPs

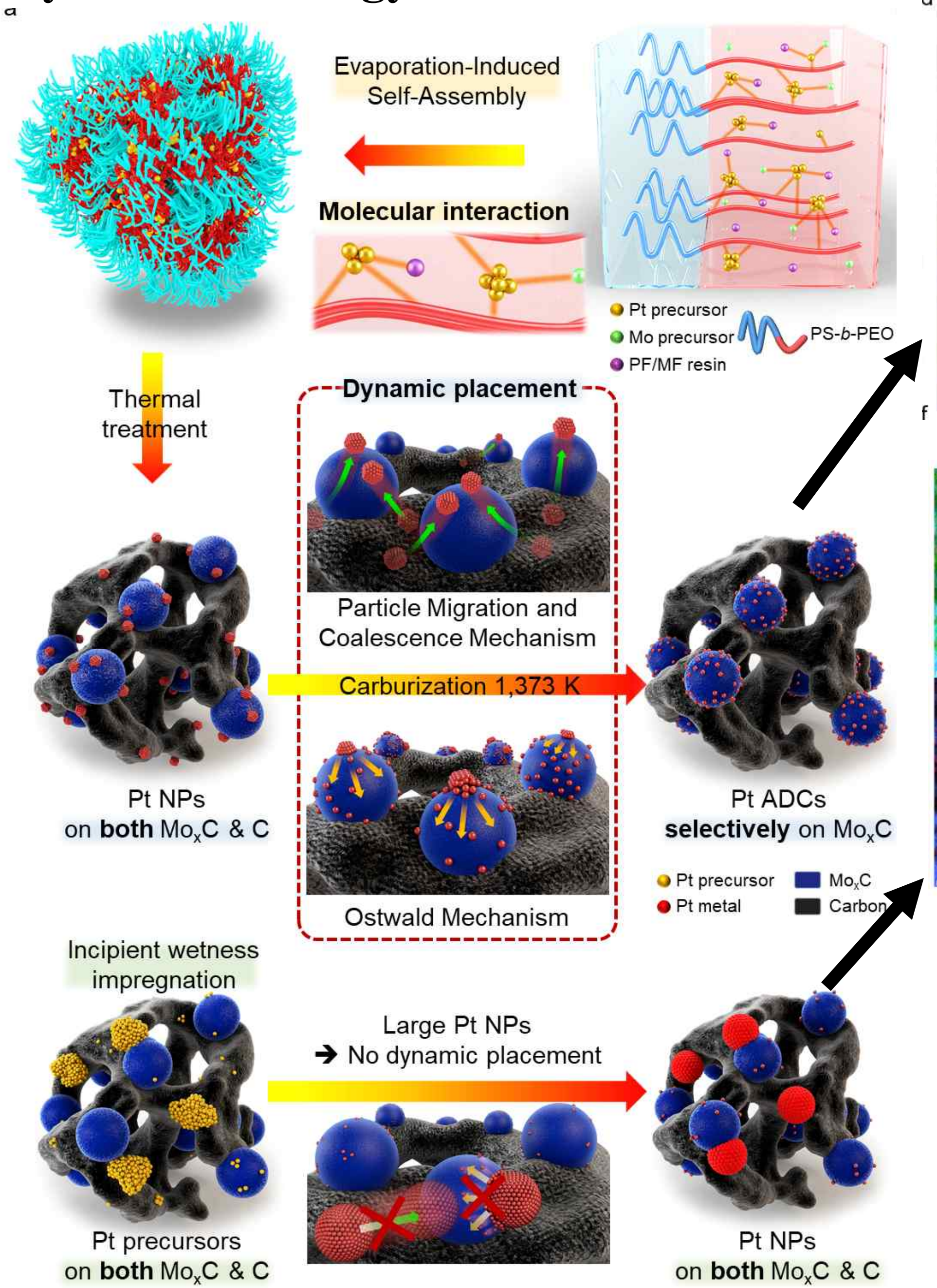
→ Selective Pt ADCs loading on Mo_xC

➔ <u>Selective loading enables the optimization of interfacial water structure</u> for Pt ADCs

Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

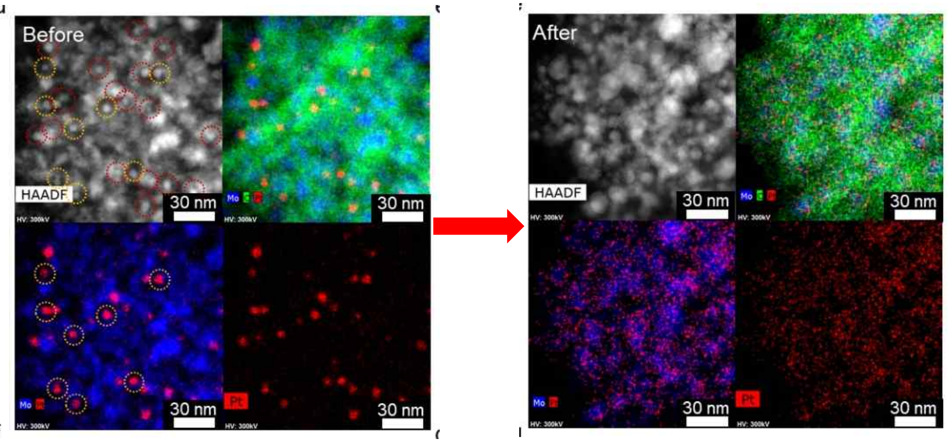
Theoretical Calculation: Hyungjun Kim at KAIST

Synthesis strategy: Molecular Interaction

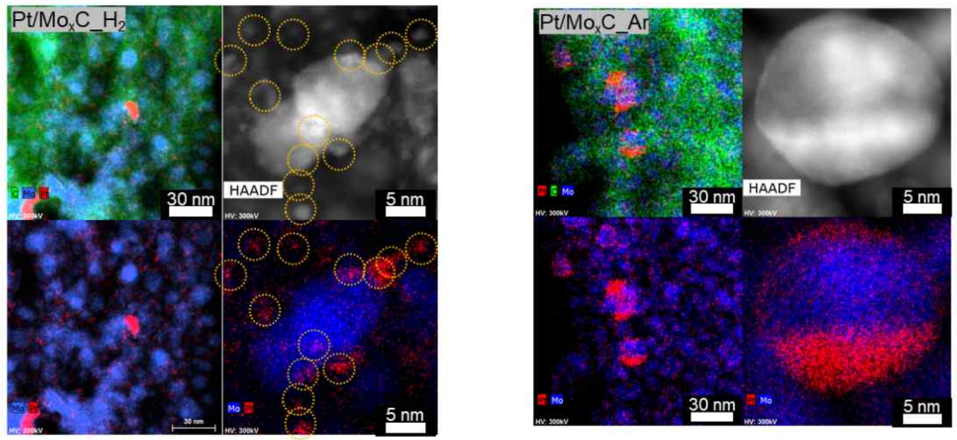


Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

EISA (Evaporation-Induced Self-Assembly)



IWI (Incipient Wetness-Impregnation)



Self-Assembly decrease the barrier for dynamic placement

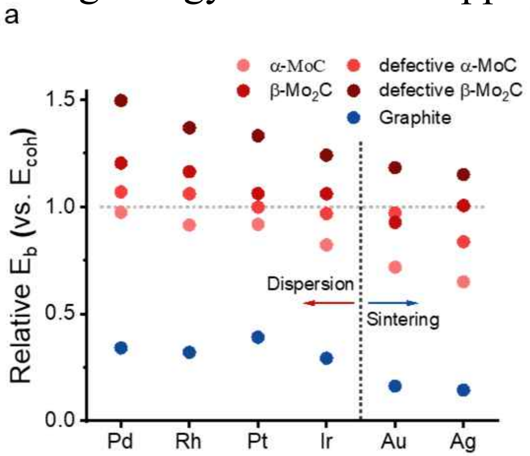
Molecular interaction between block copolymer and Precursor

→ Improve the NM distribution
(No large NM agglomerates)

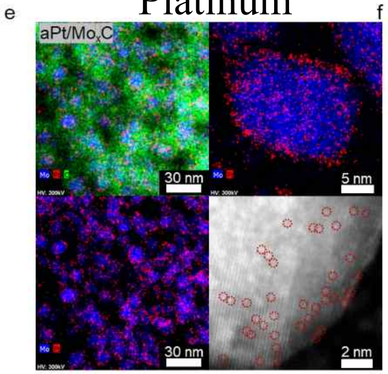
➔ Facilitate dynamic placement of NM

Versatility of dynamic placement & XAFS analysis

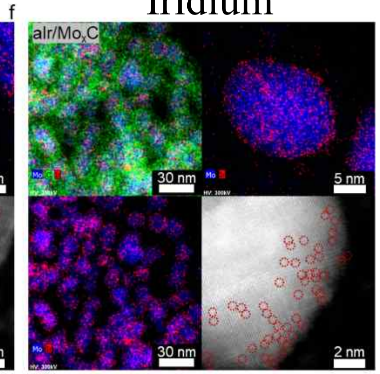
Binding energy of NM on Supports



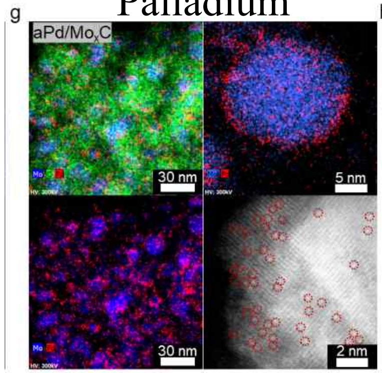
Platinum



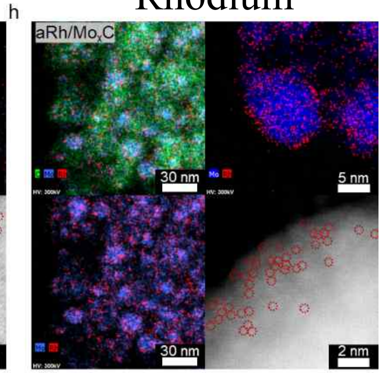
Iridium



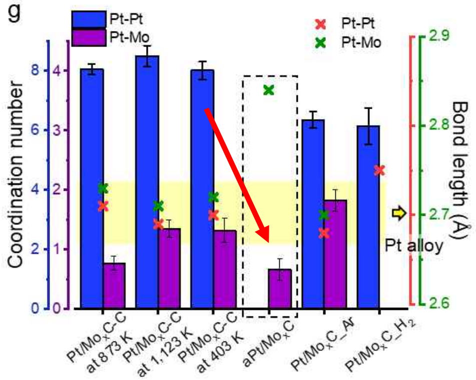
Palladium



Rhodium

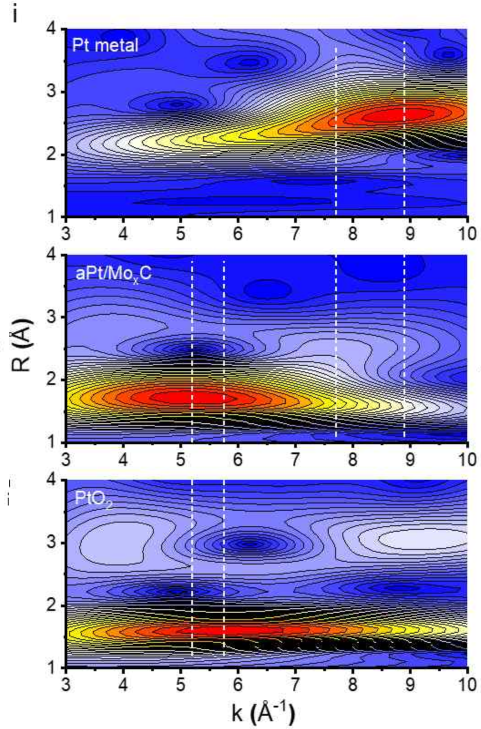


EXAFS Fitting



Pt-Pt coordination decreases

WT-EXAFS



With strong MSI of NM and Mo_xC
→ Versatile dynamic placement
(Pt, Ir, Pd, Rh)

Pt-Pt coordination decrease from ~8 to 0 after high-T dynamic placement

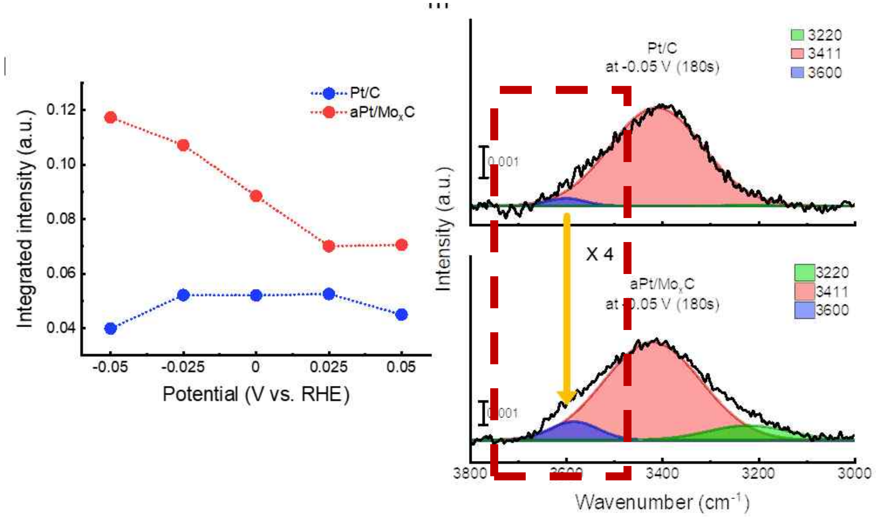
→ High-T annealing embodies dynamic placement

Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

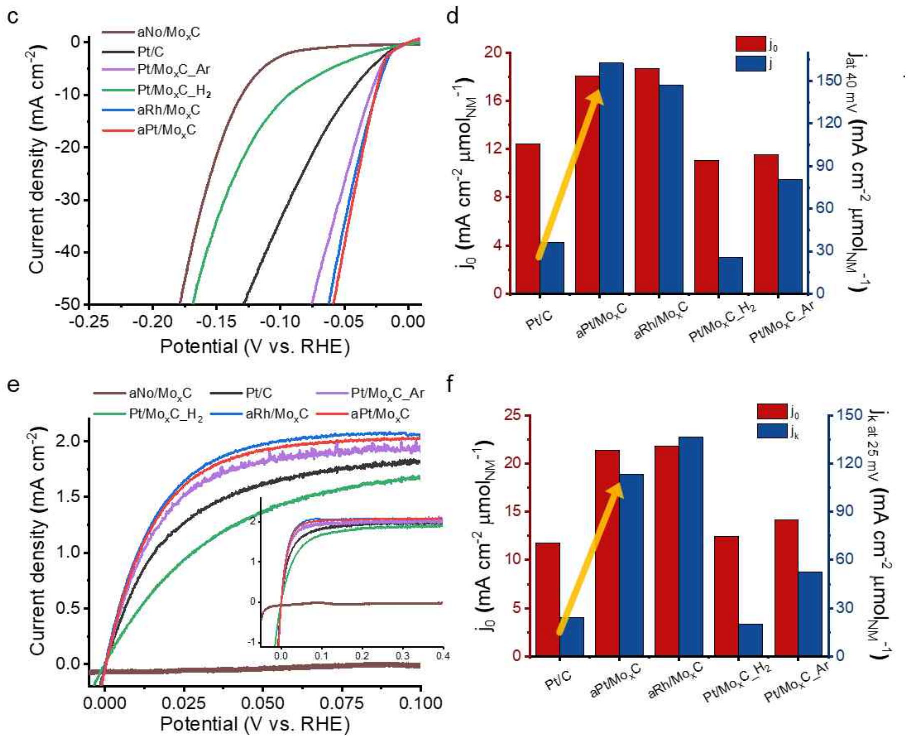
Interfacial water structure & Electrochemical performance

(Alkaline hydrogen electrocatalysis)

SEIRAS



Alkaline HER & HOR



Mo_xC supports increases the population of free water

→ Mo_xC supports decrease the water dissociation barrier

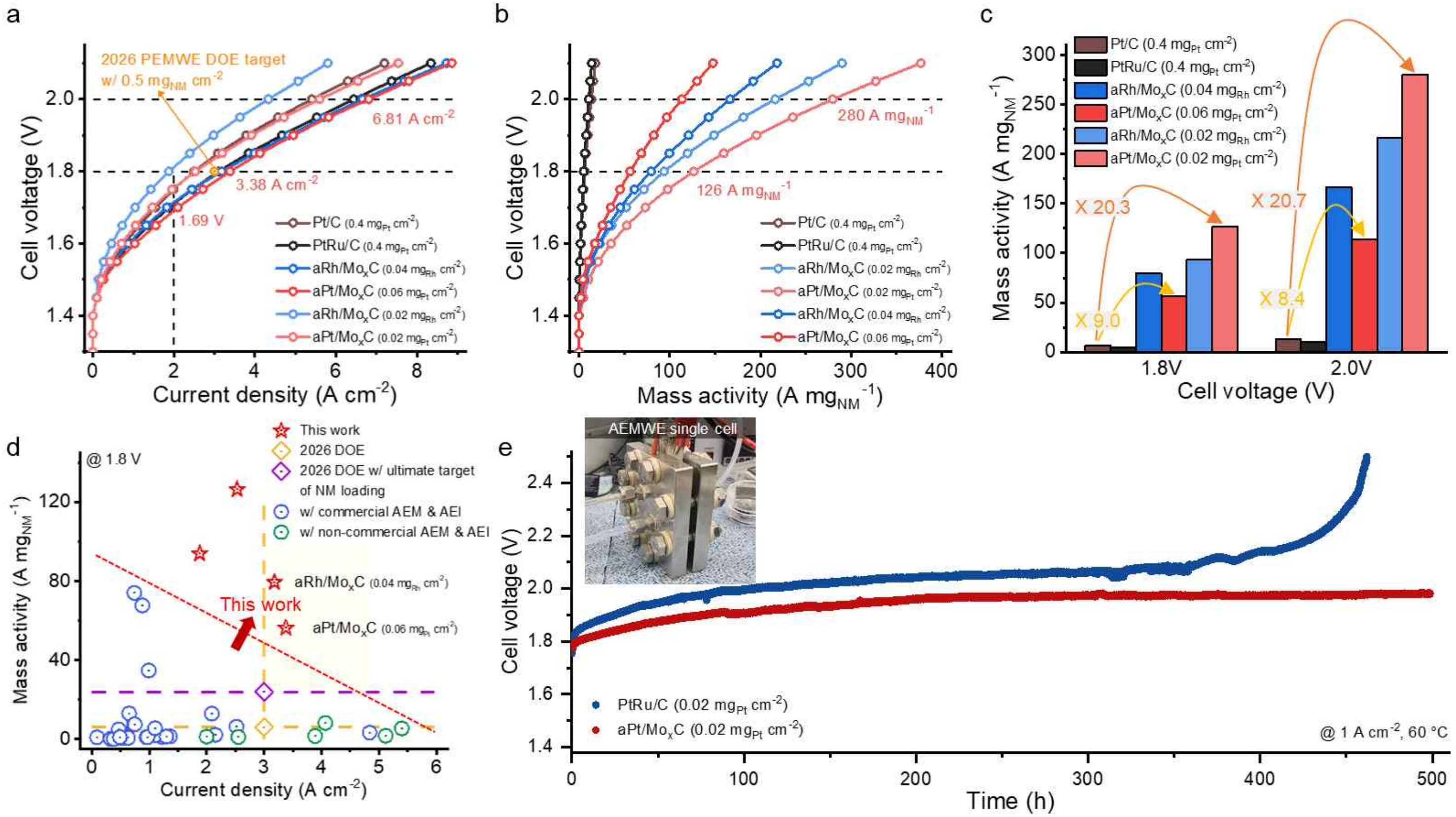
➔ Selective loading of Pt ADCs on Mo_xC supports effectively optimizes interfacial water structure for better electrokinetics for alkaline hydrogen electrocatalysis

aPt/Mo_xC (red) exhibits ~5 times higher mass activity than Pt/C (black)

➔ Increased electrokinetics of Pt by optimized interfacial water structure

Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

AEMWE performance



PEMWE DOE target

- Performance (2026): 3.0 A cm^{-2} at 1.8 V_{cell}
- NM loading (ultimate): 0.125 mg_{NM} cm^{-2}

aPt/Mo_xC: 3.38 A cm^{-2} at 1.8 V_{cell} with 0.060 mg_{Pt} cm^{-2}

- ~9 times higher mass activity than commercial Pt/C & PtRu/C
- Only aPt/Mo_xC fulfills DOE targets for PEMWE
- 500 h stability with 1 A cm^{-2}

Hyungjun Kim*& Jinwoo Lee* Energy. Env. Sci. 2025/ee/d4ee04660a

Thank you for your attention

Dr. Jong Hyun Jang (KIST)

Prof. Jeong Woo Han (SNU)

Prof. Jihan Kim (KAIST)

Prof. Segeun Jang (Kookmin Uni.)

Prof. Soo-kil Kim (Chung-Ang Uni.)

Dr. Sungjune Kim (KRICT)

NRF 한국연구재단 National Research Foundation of Korea

KETEP 한국에너지기술평가원

LOTTE CHEMICAL

KEPCO 전력연구원

LG Electronics

LG Energy Solution

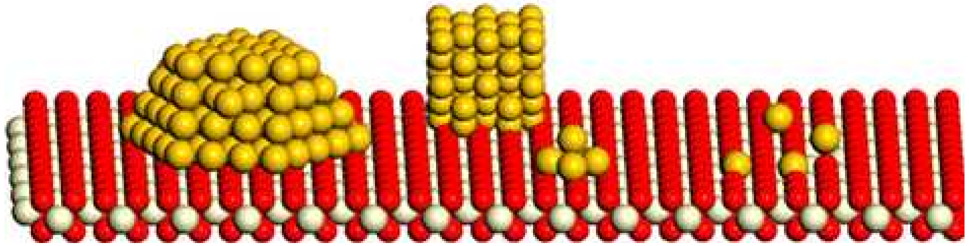
SAMSUNG ELECTRONICS

HYUNDAI NGV

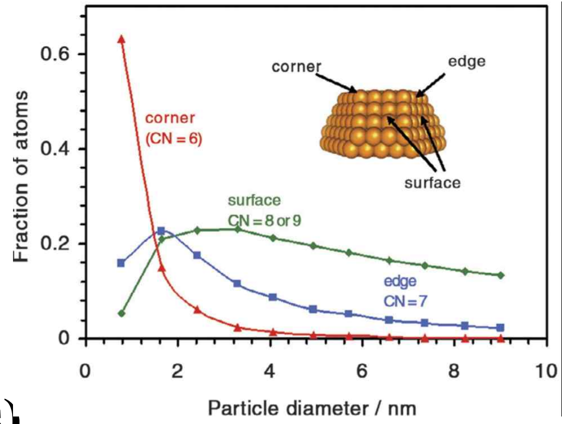
POSCO HOLDINGS

LG Chem

Requirements for low-NM AEMWE Catalysts



Chem. Rev., 2020, 120 (2) 623,

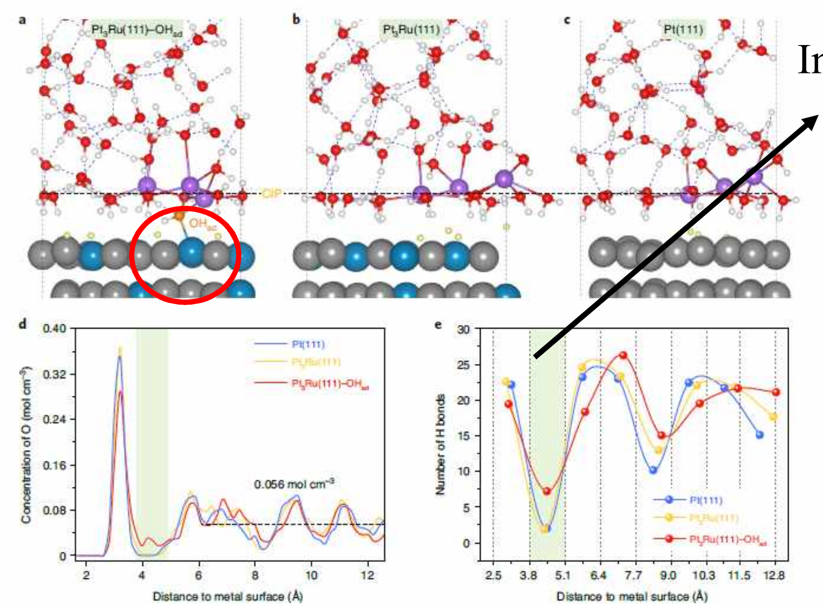


Chem. Rev., 2020, 120 (2) 623, Nanotoday, 2007, 2(4), 14

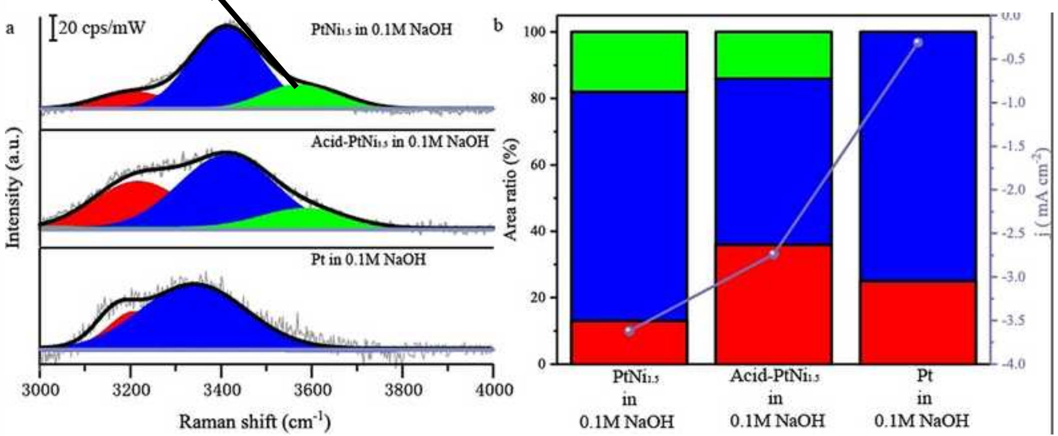
Atomically-Dispersed Catalysts (ADCs)

- Maximized NM utilization & Interfacial Active Systems

➔ Ideal platform for low-NM AEMWE



Increase of free water



Nat. Catal., 2022, 5, 900

Angew. Chem. Int. Ed., 2020, 59, 22397/

Functions of *OH species near NM active sites

- Increase of free water species (weakly H-bonded, ~3,600 cm^{-1})

➔ Optimization of Interfacial water structure → Increased water dissociation kinetics