

CLUSTER OF EXCELLENCE

Materials for **E**nergy **C**onversion and  **S**torage



Ulrike Diebold



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Günther Rupprechter
(DOR)



Leticia González

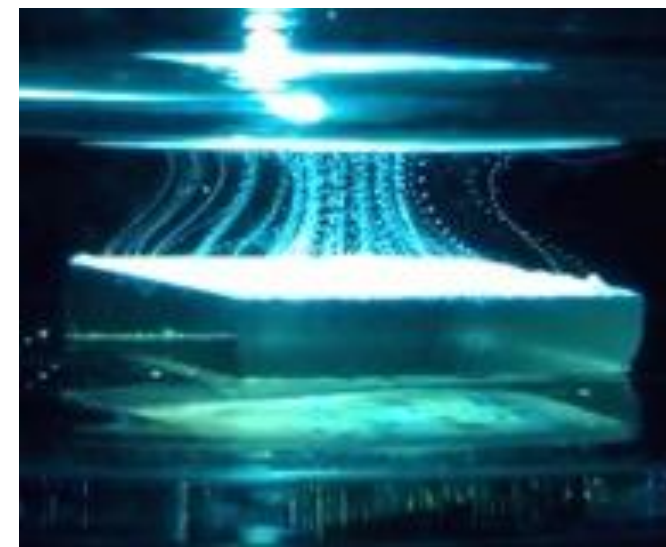
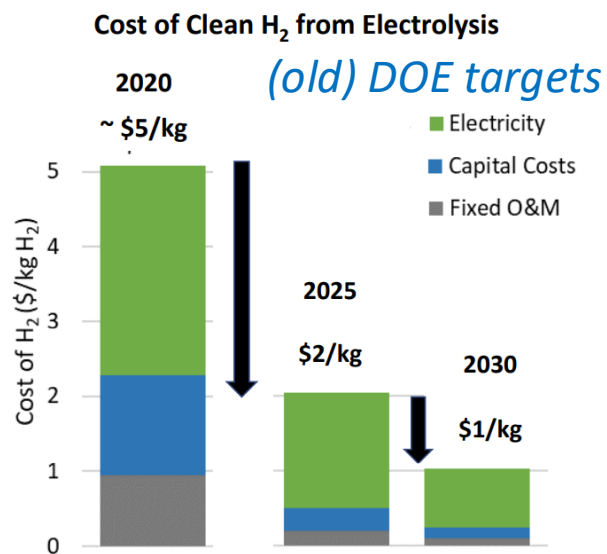
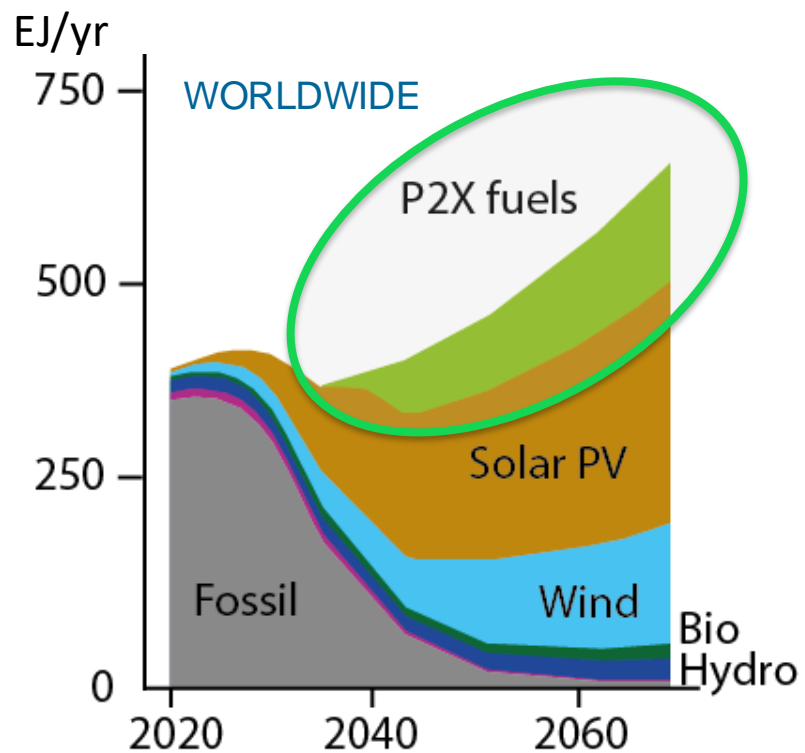


Julia Kunze-Liebhäuser



THE HARSH REALITY

- Rare expensive metals, low efficiency, not stable, or even toxic
- Despite decades of academic and industrial research: insufficient fundamental, atomistic, and mechanistic understanding of mechanism at play



Incapable to match price of conventional technologies to date (CAPEX/ OPEX)



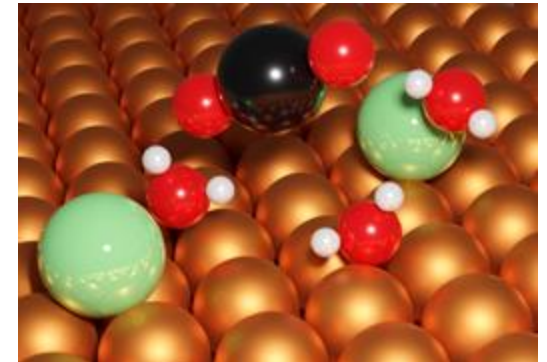
OUR RESEARCH VISION: THE ENERGY MATERIALS AGE

MECS



TAILORED COMPETITIVE SOLUTIONS FOR THE FUTURE REQUIRE:

- Atomic-level understanding of the involved processes
- Major breakthroughs in energy materials design (abundant, non-toxic, environmentally friendly, stable)
- Fundamental research enables sustainable technologies



MECS is a transformative center that is a beacon of scientific excellence
Energy storage is a worldwide challenge – needs broad expertise and capabilities!



OUR TEAM

MECS

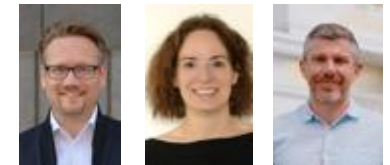


PILLAR A:
ELECTROCATALYSIS

PILLAR B:
PHOTOCATALYSIS

MECS

PILLAR C:
COMPUTATIONAL



19 outstanding PIs, 120 researchers from 5 institutions, and 45 MEuro with complementary expertise in physics, chemistry, materials science

The nucleus for synergies in Austria and internationally creates a unique network for energy conversion technology



FOCUS: ELECTROCATALYSIS

CHALLENGES

- Conversion of H_2O and CO_2 with high **energy efficiency**
- **Selective** formation of **fuels** and **value-added chemicals**:
 H_2 , hydrocarbons, alcohols, ...
- Catalyst development (MoS_2 , W_2C , Ni-C) and material (e.g. membrane) **stability in electrolyzers**

APPROACH

- Study **catalysts in operation** (*operando*) by spectroscopy, microscopy, diffraction
- New **cross-disciplinary experimental** approaches
- Strong interaction with **computational modeling**

TASK LEADERS & TEAM



Kunze-Liebhäuser

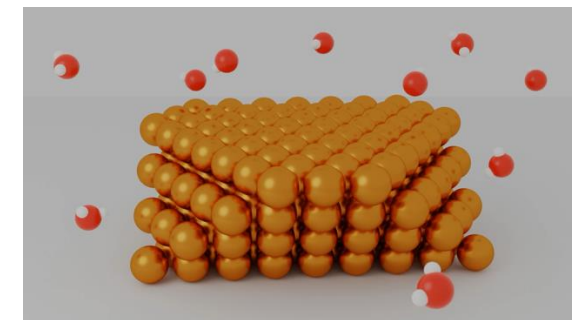


TU WIEN Fleig



SOLID / LIQUID INTERFACE (LOW T)

□ CATALYST SURFACE & ELECTROLYTE

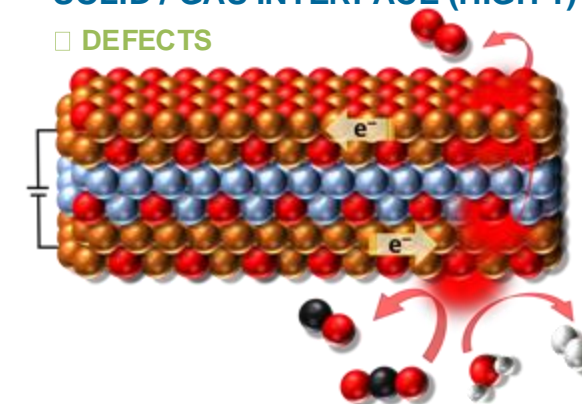


Kunze, *Nature Catalysis* 2021

W_2C : Kunze/Valtiner, *Angewandte* 2025 just accepted

SOLID / GAS INTERFACE (HIGH T)

□ DEFECTS



Fleig/Opitz in *Nature Commun.* 2020



FOCUS: COMPUTATIONAL MODELING & MATERIALS SIMULATIONS

CHALLENGES

- Model complex catalytic processes on the mesoscale under realistic conditions

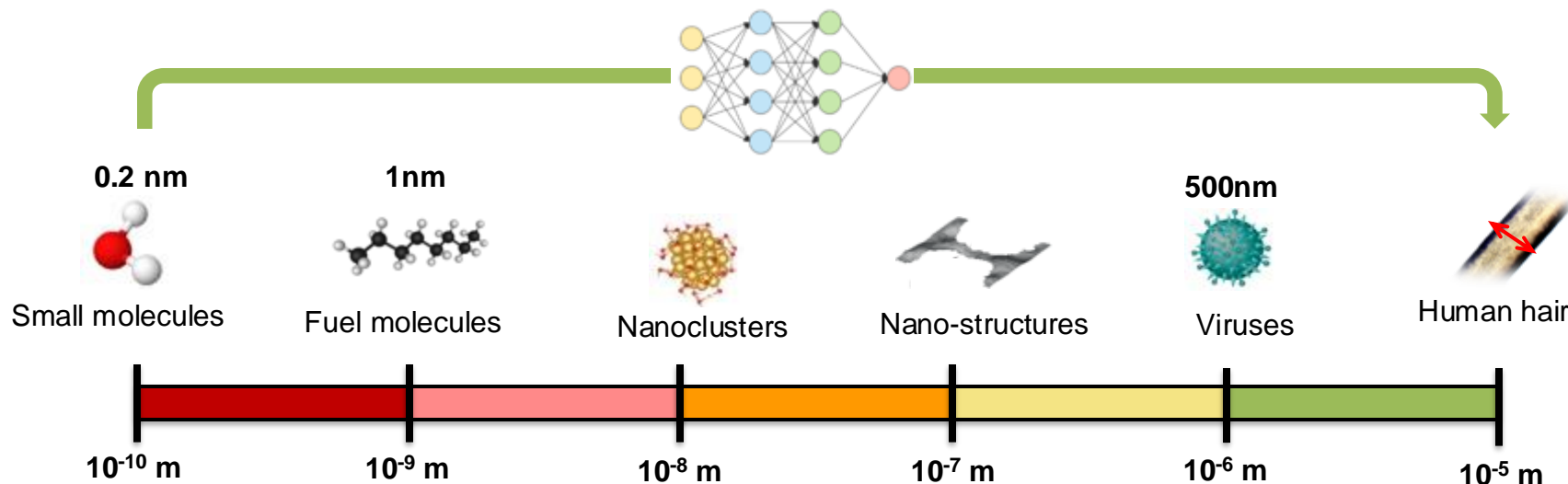
APPROACH

- Use quantum mechanics and scale the results to the μm regime (millions of atoms) via machine learning
- Upscaling to stack level

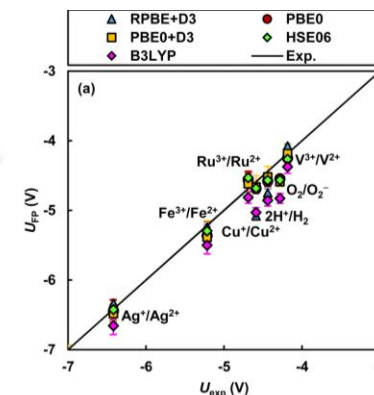
Quantum mechanics - Schrödinger equation

$$H\Psi = i\hbar \frac{d}{dt} \Psi$$

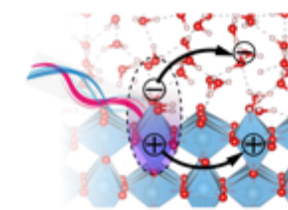
Predicts the behavior of atoms and individual electrons



Electro and photocatalysis



Temperature, light, and current



TASK LEADERS & TEAM



Kresse



Madsen

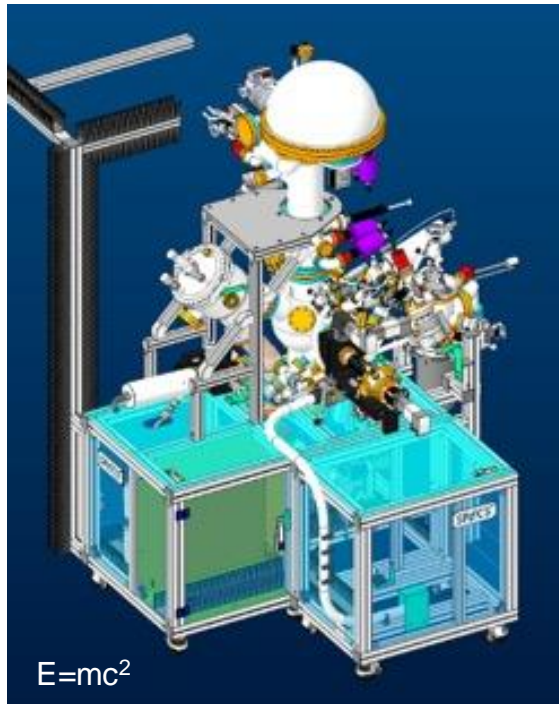




LARGE RESEARCH INFRASTRUCTURE INVESTMENT WITHIN MECS AND CONSORTIUM



MECS CORE FACILITY



E=mc²

ENERGY MATERIALS CHARACTER CENTER

Single crystals
thin films,
powders
UHV to mbar
LN₂ to HT
NAP-XPS, -UPS,
TPD, MS.



IN SITU ELECTRON MICROSCOPY

Dedicated MEMS cells for in situ electrochemical gas and liquid phase studies.



AUSTRIAN SUPERCOMPUTING FACILITIES

VIENNA SCIENTIFIC CLUSTER 4/5
VSC4/5
MUSICA GPU Cluster



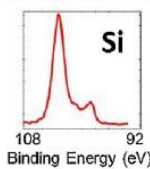
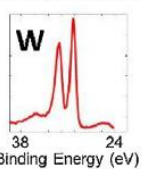
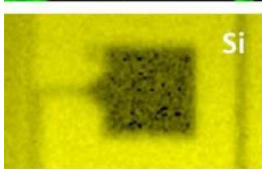
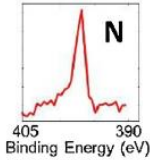
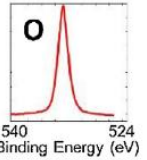
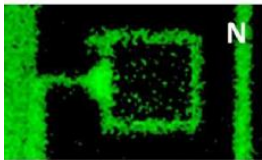
Quasi in-situ operation of all equipment (unique lab & combination of EC-analysis)



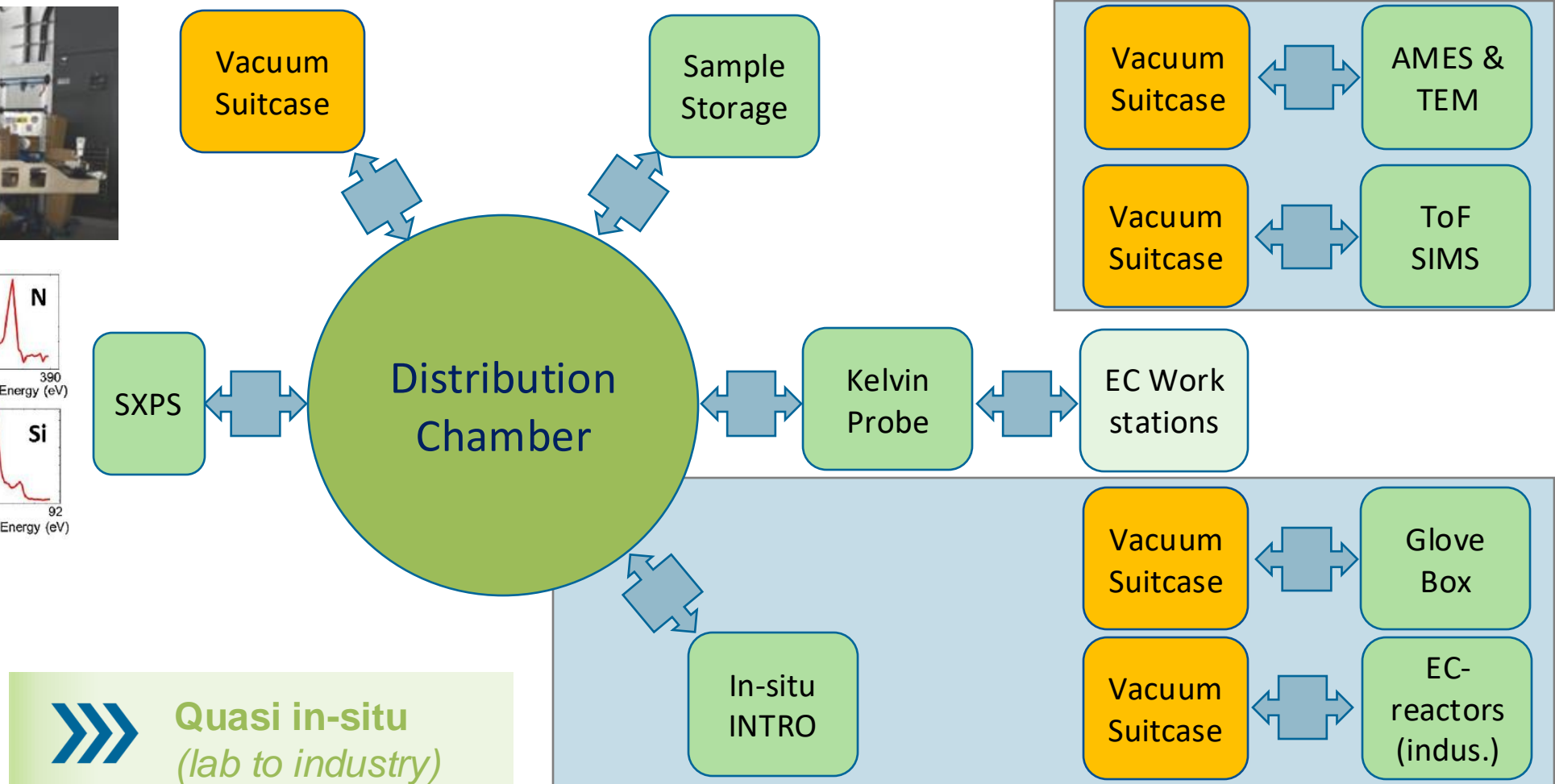
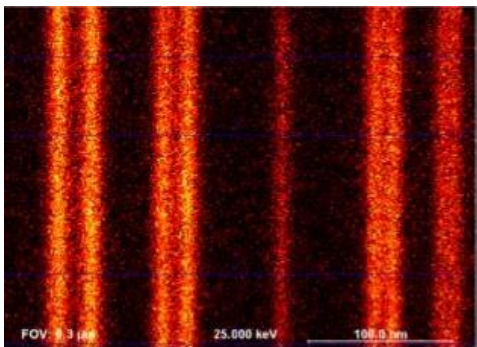
LARGE RESEARCH INFRASTRUCTURE INVESTMENT WITHIN MECS AND CONSORTIUM



SXPS



AMES

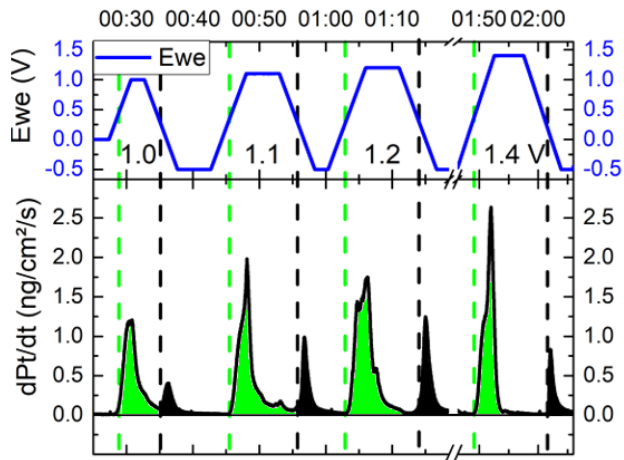




Real time catalyst stability

(example Pt)

W₂C: Kunze/Valtiner, Angewandte 2025 just accepted
ACS Applied Materials & Interfaces 12 (46), 51530-51536



- Real time analysis of electrolytes
- Catalyst degradation mechanism

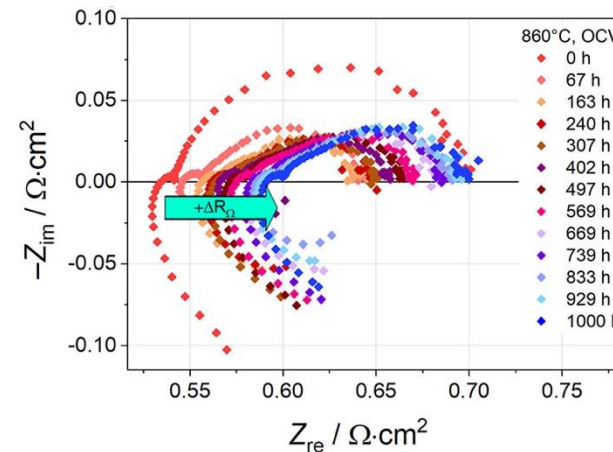
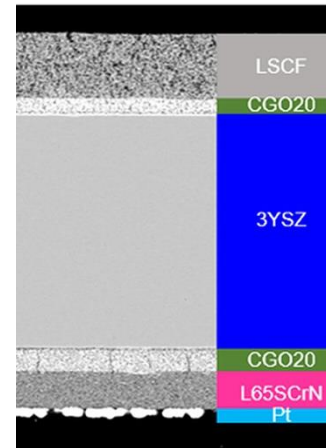
Prof. M. Valtiner/ Prof. J. Kunze

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julia.kunze@uibk.ac.at

Long term stability of HT electrolysis full cells

(example perovskite-chromite SOEC)

ACS Applied Energy Materials 5 (7), 8143-8156



- Temperature dependent electrochemistry at high temperature
- Perovskite solid state electrolytes

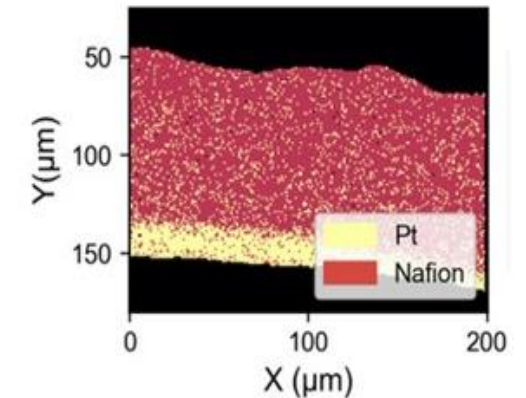
Prof. A. Opitz and Prof. J Fleig

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Stack level migration of ions

(example Pt/Nafion)

Advanced Energy and Sustainability Research
2024 5 (9), 2400048



- Synchrotron based X-ray fluorescence at stack level
- Synchrotron operando EC

Prof. T. Sheppard (new at TUW)

thomas.sheppard@tuwien.ac.at

MECS | CLUSTERING EXCELLENCE

5-7th May 2025: 4th COAST conference at TU Wien (sign up at <https://coe-mecs.at/coast2025>)

Q1/2026: Opening of MECS.labs in Vienna as **hub between science and industry** (follow us on social media)

 COE MECS

 COE MECS
(soon on bluesky)

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Innovating for a Sustainable Future.

MECS.labs

...thanks for your attention