



The Integrated Fuel & Chemical Science Center

Adaptive Conversion Systems for Sustainable Energy Carriers and Chemicals
Renewal Proposal EXC2186

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Nomenclature

Acronyms and abbreviations

5-HMF	5-hydroxymethylfurfural
AEM	anion exchange membrane
AESA	absolute environmental sustainability assessment
AI	artificial intelligence
AOR	ammonia oxidation reaction
AR	Associated Researcher
AST	accelerated stress test
BCY	yttrium-doped barium cerate
BCZY	yttrium-doped barium zirconate-cerate
BECCU	bio-energy conversion with carbon capture and utilization
BMBF	Federal Ministry of Education and Research
BPM	bipolar membrane
BZY	yttrium-doped barium zirconate
CA	Competence Area
CA1	Competence Area 1
CA2	Competence Area 2
CA3	Competence Area 3
CCC-NEMD	Chemical-Color-Coded Non-equilibrium molecular dynamics
CCO	Chief Communication Officer
CEM	cation-exchange membrane
CEMC	cluster-expansion method calculations
CFO	Chief Financial Officer
CMP	Center for Mobile Propulsion
CNF	carbon nanofiber
CNT	carbon nanotubes
CO ₂ RR	electrocatalytic carbon dioxide reduction
CoE	Cluster of Excellence
COO	Chief Operating Officer
CR	compression ratio
CTF	covalent triazine frameworks
CTY	ChemTraYzer
CVC	constant volume chamber
CYA	Center for Young Academics
DAC	direct air capture
DAFC	direct ammonia fuel cell
DFG	Deutsche Forschungsgemeinschaft
DFT	density functional theory

Acronyms and abbreviations

DLFC	direct liquid fuel cell
DMP	data management plans
DNS	direct numerical simulation
DSM	demand-side management
EATS	exhaust after-treatment system
EBCC	ethanol-2-butanone-cyclopentanone-cyclopentane
EC-RTMS	electrochemical real-time mass spectrometry
EGR	exhaust gas recirculation
EIS	electrochemical impedance spectroscopy
ESM	energetic span model
EU	European Union
FAIR	Findable, Accessible, Interoperable, Reusable
FCDF	Fuel & Chemical Design Forum
FCDP	Fuel & Chemical Design Process
FDCA	furandicarboxylic acid
FIB-SEM	focused ion beam - scanning electron microscopy
FSC	The Fuel Science Center
FSC ²	The Integrated Fuel & Chemical Science Center
FTIR	Fourier-transform infrared spectroscopy
FZJ	Forschungszentrum Jülich
GCE-DFT	grand canonical ensemble density functional theory
GCMS	gas chromatography and mass spectrometry
GDC	gadolinium-doped ceria
GHG	greenhouse gas
HAA	3-(3-hydroxyalkanoyloxy)alkanoic acid
HC	hydrocarbon
HR	high reactivity
HS	high-swirl
HT	high-tumble
HyFIT	hydroformylated Fischer-Tropsch
IAB	International Advisory Board
ICCC	integrated carbon capture and conversion
ICE	internal combustion engine
ICNP	iron carbide nanoparticle
IDT	ignition delay time
ifeu	Institut für Energie- und Umweltforschung Heidelberg gGmbH
IPPR	internal peer project review
IR	infrared
ITMC	Institute of Technical and Macromolecular Chemistry
JARA	Jülich Aachen Research Alliance
JPI	Junior Principal Investigator

JRG	junior research group
KEAA	ketone-esters-alcohol-alkanes
LAS	laser absorption spectroscopy
LBV	laminar burning velocity
LCA	life-cycle assessment
LES	large eddy simulation
LIF	laser-induced fluorescence
LR	low reactivity
LTT	Chair of Technical Thermodynamics
MBFC	microbial fuel cell
MC	main chamber
MCCS	molecularly controlled combustion system
MCPS	molecularly controlled propulsion system
MCR	multivariate curve resolution
MD	molecular dynamics
MDH	methanol dehydrogenase
MFA	material flow analysis
MHBF	multifunctional high-pressure burner facility
ML	machine learning
MPI CEC	Max Planck Institute for Chemical Energy Conversion
MRI	magnetic resonance imaging
MS	molecular spark
MT	molecular torch
MW	microwave
NDIR	non-dispersive infrared
NGP ²	Center for Next Generation Processes and Products
NHC	N-heterocyclic carbene
NLP	natural language processing
NMR	nuclear magnetic resonance
NVP	N-vinyl-2-pyrrolidone
OER	oxygen evolution reaction
ORR	oxygen reduction reaction
PC	pre-chamber
PEMFC	proton exchange membrane fuel cell
PFAS	per- and polyfluoroalkyl substances
PFSA	perfluorosulfonic acid
PI	Principal Investigator
PIV	particle image velocimetry
PM	particulate matter
PNFA	process network flux analysis
PU	Polyurethane

Symbols

QM	quantum mechanics
RCM	rapid compression machine
RDM	research data management
RDMO	research data management organizer
rGO	reduced graphene oxide
rSOC	Reversible Solid Oxide Cell
RWTH	RWTH Aachen University
s/D ratio	stroke/bore ratio
SAR	specific absorption rate
SCE	single cylinder engine
SCR	selective catalytic reduction
SOFC	Solid Oxide Fuel Cell
SPCFC	solid proton-conducting fuel cell
SRA	Strategic Research Area
SRA-AFU	SRA “Ammonia Fuel Utilization”
SRA-CFA	SRA “Carbon-based Fuel Application”
SRA-CSP	SRA “Concatenated Synthetic Pathways”
SRA-RACS	SRA “Resilient & Adaptive Conversion Systems”
SRA-TCP	SRA “Translational Catalytic Processes”
ST	shock tube
TCR	turbulent compression reactor
TDA	Toluene diamine
TEM	transmission electron microscopy
TMFB	Tailor-Made Fuels from Biomass
TPMS	triply periodic minimal surfaces
TRT	Translational Research Team
UDE	universal differential equations
XCT	X-ray computed tomography
XRD	X-ray diffraction
YSZ	yttrium-stabilized zirconia

Symbols

η_i net indicated efficiency

1 General data

1.1 Title in German and English

The Integrated Fuel & Chemical Science Center

Adaptive Umwandlungssysteme für erneuerbare Energieträger und Chemikalien

Adaptive Conversion Systems for Sustainable Energy Carriers and Chemicals

1.2 Applicant university/universities

Managing University
RWTH Aachen University (RWTH)

1.3 Spokesperson(s)

Authorised Spokesperson of the Managing University	
Prof. Dr.-Ing. (USA) Stefan Pischinger	
Further spokesperson	Institutions
Prof. Dr. rer. nat. Walter Leitner	RWTH Aachen University
	Max Planck Institute for Chemical Energy Conversion

1.4 Participating Institutions

Participating institutions	Location
Forschungszentrum Jülich (FZJ)	Jülich
Max Planck Institute for Chemical Energy Conversion (MPI CEC)	Mülheim a. d. R.

1.5 Principal Investigators

No.	Principal Investigators	Location/ Institution	Field of Expertise	Position
1	Jun.-Prof. Dr. phil. Katrin Arning*	Aachen, RWTH	Risk Perception and Communication	W1 tenure track
2	Univ.-Prof. Dr.-Ing. Dipl.- Wirt.Ing. Niklas von der Aßen*	Aachen, RWTH	Technical Thermodynamics	W3 permanent
3	Univ.-Prof. Dr.-Ing. Lars M. Blank	Aachen, RWTH	Applied Microbiology	W3 permanent
4	Prof. Dr. rer. nat. habil. Rüdiger Eichel	Jülich, FZJ	Fundamental Electrochemistry	W3 permanent
		Aachen, RWTH	Material and Process of Electrochemical Energy Storage and Conversion	
5	Univ.-Prof. Dr. Kathrin Greiff*	Aachen, RWTH	Anthropogenic Material Cycles	W3 permanent
6	Univ.-Prof. Dr. rer. nat. Sonja Herres-Pawlis*	Aachen, RWTH	Bioinorganic Chemistry	W3 permanent
7	Univ.-Prof. Dr.-Ing. Karl Alexander Heufer	Aachen, RWTH	High Pressure Gas Dynamics	W3 permanent
8	Univ.-Prof. Dr.-Ing. Andreas Jupke	Aachen, RWTH	Fluid Process Engineering	W3 permanent
		Jülich, FZJ	Integrated Bio-Refineries	
9	Univ.-Prof. Dr. rer. nat. Jürgen Klankermayer	Aachen, RWTH	Translational Molecular Catalysis	W3 permanent
10	Univ.-Prof. Dr. rer. nat. habil. Lars Lauterbach*	Aachen, RWTH	Synthetic Microbiology	W2 permanent

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1 General data

(Continued)

No.	Principal Investigators	Location/ Institution	Field of Expertise	Position
11	Univ.-Prof. Dr. phil. Carmen Leicht-Scholten*	Aachen, RWTH	Gender and Diversity in Engineering	W2 permanent
12	Univ.-Prof. Dr. rer. nat. Walter Leitner	Aachen, RWTH	Technical Chemistry and Petrochemistry	W3 permanent
		Mühlheim a.d.R., MPI CEC	Molecular Catalysis	
13	Prof. Dr. techn. Karl Mayrhofer*	Erlangen, FZJ	Electrocatalysis	W3 permanent
14	Univ.-Prof. Dr. rer. nat. Anna Mechler*	Aachen, RWTH	Electrochemical Reaction Engineering	W2 temporary
		Jülich, FZJ	Energy Technologies	
15	Univ.-Prof. Alexander Mitsos, Ph.D.	Aachen, RWTH	Process Systems Engineering	W3 permanent
		Jülich, FZJ	Energy Systems Engineering	
16	Univ.-Prof. Dr. rer. nat. Regina Palkovits	Aachen, RWTH	Heterogeneous Catalysis and Chemical Technology	W3 permanent
		Jülich, FZJ	Sustainable Hydrogen Economy	
17	Univ.-Prof. Dr.-Ing. (USA) Stefan Pischinger	Aachen, RWTH	Thermodynamics of Mobile Energy Conversion Systems	W3 permanent
18	Univ.-Prof. Dr.-Ing. Heinz Pitsch	Aachen, RWTH	Combustion Technology	W3 permanent
19	Univ.-Prof. Dr. rer. nat. Dörte Rother	Jülich, FZJ	Synthetic Enzyme Cascades	W3 permanent
		Aachen, RWTH		
20	Univ.-Prof. Dr. Franziska Schoenebeck	Aachen, RWTH	Organic Chemistry	W3 permanent
21	Univ.-Prof. Dr. rer. nat. Ulrich Simon	Aachen, RWTH	Inorganic Chemistry and Electrochemistry	W3 permanent
22	Prof. Dr. Siegfried R. Waldvogel*	Mühlheim a.d.R., MPI CEC	Electrosynthesis	W3 permanent
23	Univ. Prof. Dr. rer. pol. Grit Walther	Aachen, RWTH	Operations Management	W3 permanent
24	Univ.-Prof. Dr.-Ing. Matthias Wessling	Aachen, RWTH	Chemical Process Engineering	W3 permanent
25	Univ.-Prof. Dr. rer. nat. Mirjam Zobel*	Aachen, RWTH	Crystallography and X-Ray Spec- troscopy	W3 permanent

10 principal investigators are women; this is a share of 40 percent.

* principal investigators not indicated as principal investigators in the establishment proposal

1.6 Cooperation partners

No.	Institutional cooperation partners	Location
1	University of Alberta	Edmonton, Canada
2	University of California	Berkeley/Los Angeles /Santa Barbara, USA
3	ifeu - Institut für Energie- und Umweltforschung	Heidelberg, Germany
4	NRW.Energy4Climate	Düsseldorf, Germany
5	ETH Zürich	Zürich, Switzerland

2 Summary of the proposal

2.1 English (max. 3000 characters incl. spaces)

The future will be renewable! Shaping a post-fossil era mandates the development of disruptive technologies for the production and use of liquid energy carriers and chemical products as basis for a truly sustainable energy-chemistry nexus within the planetary boundaries. Energy-rich molecules – harnessing renewable energy electrochemically or via green hydrogen with renewable feedstocks – offer an important contribution to the “defossilization” of the transport sector, especially for long-haul, heavy duty, and non-road applications, which are difficult or even impossible to electrify. At the same time, they are essential components for a net-zero or even CO₂-negative production of chemicals serving as the foundation for nutrition, health, and prosperity.

In this complex and highly dynamic context, FSC² generates fundamental knowledge and novel scientific methods for the development of adaptive technical solutions to valorize renewable electricity and feedstocks into liquid energy carriers and chemicals in a systems approach. Based on previous achievements, the integral rather than competitive use of renewable electricity together with feedstocks from atmospheric, biogenic, and industrial sources forms the basis of the FSC² design framework for “bio-hybrid fuels and chemicals”. Nitrogen-based substances such as ammonia are newly included to critically assess their potential as molecular energy carriers and chemical building blocks. In addition to thermal energy conversion, electro-chemical devices for recuperating chemically stored energy are studied and the applicability of molecular controlled combustion systems to existing vehicle is considered. Novel concatenated synthetic pathways and translational catalytic processes for the (co-)production of fuels and chemicals are explored and validated. Resilient and adaptive fuel & chemical conversion systems are designed in an integrated approach bridging scales from molecule to supply chains.

RWTH Aachen University (RWTH) and its strategic partners Forschungszentrum Jülich (FZJ) and Max Planck Institute for Chemical Energy Conversion (MPI CEC) are ideally positioned to establish an integrated research center able to adapt its research framework continuously to new directions. The research activities are organized in five Strategic Research Areas (SRAs) integrating individual project work in a dynamic teams approach, embracing diversity on all levels as a major driver for creativity. Establishing 5 junior research groups and mentoring programs for early-stage researchers contributes to attractive career opportunities ranging from academic trajectories to entrepreneurship. FSC² will catalyze strategic developments at the partner institutions by 12 strategic appointments including new and inter-institutional professorships.

2 Summary of the proposal

2.2 German (max. 3000 characters incl. spaces)

Die Zukunft wird erneuerbar sein! Die Gestaltung eines postfossilen Zeitalters erfordert die Entwicklung disruptiver Technologien zur Herstellung und Nutzung von flüssigen Energieträgern und chemischen Produkten als Grundlage für eine nachhaltige Schnittstelle von Energie- und Chemie. Energiereiche Moleküle, die erneuerbare Energien elektrochemisch oder über grünen Wasserstoff zusammen mit nachwachsenden Rohstoffen speichern, leisten einen wichtigen Beitrag zur "Defossilisierung" des Transportsektors, insbesondere für schwierig elektrifizierbare Schwerlast- und Non-Road-Anwendungen. Gleichzeitig sind sie wesentliche Bestandteile für eine Netto-Null- oder sogar CO₂-negative Produktion von Chemikalien, die die Grundlage für Ernährung, Gesundheit und Wohlstand darstellen.

In diesem komplexen und hochdynamischen Kontext generiert The Integrated Fuel & Chemical Science Center (FSC²) grundlegendes Wissen und neue wissenschaftliche Methoden zur Entwicklung adaptiver technischer Lösungen zur Verwertung von erneuerbarer Elektrizität und Rohstoffen für flüssige Energieträger und Chemikalien in einem Systemansatz. Basierend auf den bisherigen Errungenschaften bildet die integrale Nutzung von erneuerbarem Strom zusammen mit Rohstoffen aus atmosphärischen, biogenen und industriellen Quellen die Grundlage des FSC²-Designrahmens für "bio-hybrid fuels and chemicals". Stoffe auf Stickstoffbasis wie z. B. Ammoniak werden nun mit einbezogen, um deren Potenzial als molekulare Energieträger und chemische Bausteine zu analysieren. Neben thermischen werden auch elektrochemische Energiewandler zur Rückgewinnung chemisch gespeicherter Energie untersucht, und die Anwendung molekular kontrollierter Brennverfahren für existierende Fahrzeuge angestrebt. Neuartige, verkettete Synthesewege und translationale katalytische Prozesse für die (Co-)Produktion von Kraftstoffen und Chemikalien werden in einem gesamtheitlichen Ansatz entwickelt, der die Skalen vom Molekül bis zur gesamten Lieferkette überbrückt. Produktionsprozesse und energetische Nutzung bilden die Säulen eines resilienten Gesamtsystems.

Die RWTH Aachen University (RWTH) und ihre strategischen Partner Forschungszentrum Jülich (FZJ) und Max-Planck-Institut für Chemische Energiekonversion sind ideal aufgestellt, um ein integriertes Forschungszentrum zu etablieren, das sein Forschungsprofil kontinuierlich an neue Richtungen anpasst. Die Forschungsaktivitäten sind in 5 Strategic Research Areas (SRAs) organisiert, die individuelle Projektarbeit in einem dynamischem Team Ansatz integrieren, der Diversität auf allen Ebenen als wesentlichen Treiber für Kreativität miteinschließt. Die Einrichtung von 5 Nachwuchsgruppen und Mentoring-Programmen eröffnet attraktive Karrieremöglichkeiten. FSC² wird die strategische Entwicklung an den Partnerinstitutionen durch 12 Berufungen unterstützen, darunter sowohl neue als auch institutsübergreifende Professuren.

3 Objectives of the Cluster of Excellence

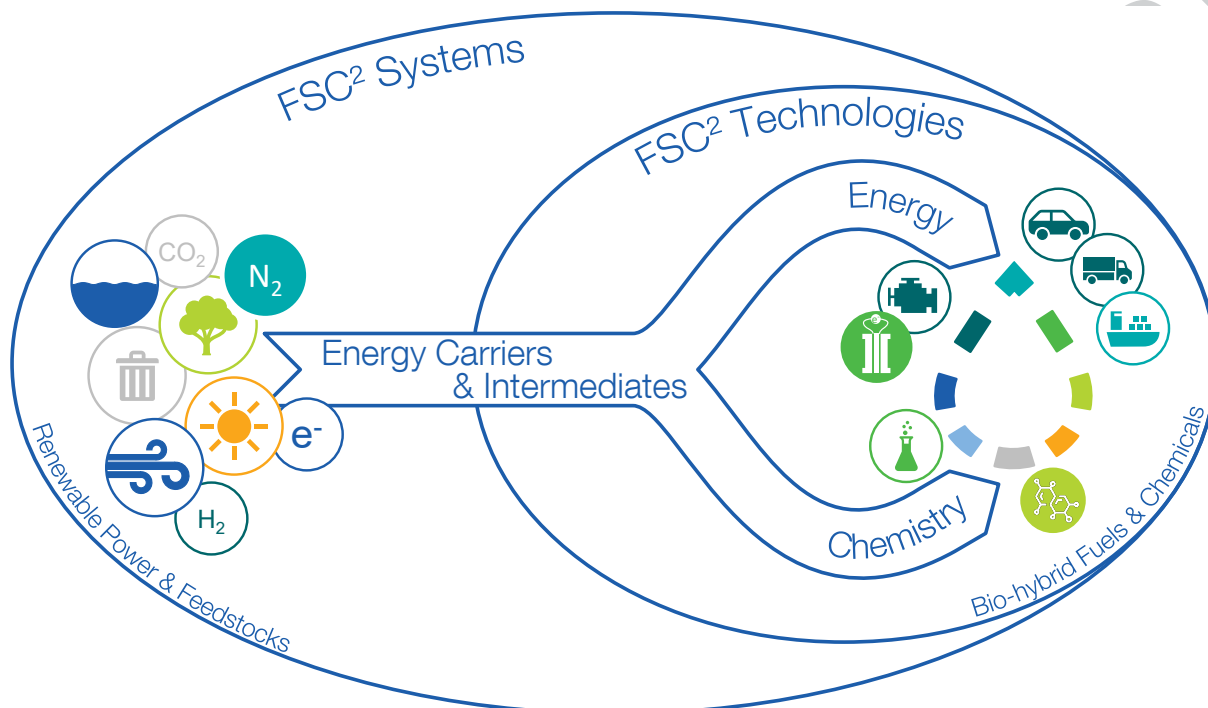
3.1 Background and Motivation

The urgently required reduction of greenhouse gas emissions, especially CO₂, has led to extensive worldwide efforts aiming at net-zero and even carbon negative technologies. The deployment of renewable power generation is rapidly growing, mainly through installation of wind turbines and photovoltaic systems as cost-effective technologies for electricity generation [231]. At the present time, biomass still provides the highest share of renewable energy and – albeit limited in availability – will remain an important component also in the future [231]. With both green electricity and biomass being highly fluctuating and delocalized resources, the dominating challenge for a global system based on renewable energy is its transportation and storage for effective use in the specific sectors of application [232].

Energy rich molecules – generated electrochemically or *via* green hydrogen or biomass – offer a key solution due to the high energy content of their chemical bonds resulting in high volumetric and gravimetric energy density in liquid form. The integration of such **energy carriers and chemical intermediates** into the sectors transport/mobility and chemical production holds major opportunities to “defossilize” these areas that are currently based almost exclusively on crude oil and responsible for a total of 24 % of the anthropogenic CO₂ emissions [233]. Synthetic hydrocarbons, methanol, and ammonia are emerging as promising options. Technologies for their generation from the abundant feedstocks water, nitrogen, CO₂ and biomass are demonstrated and deployed worldwide at rapidly increasing rates [231]. Their use – directly or in upgraded form – as **fuels in thermal or electrochemical energy conversion systems** complements the direct electrification and use of hydrogen for powertrains in the transport and mobility sector. At the same time, they provide entry points into **existing value chains and new production pathways for chemical products** as an essential pillar for a closed anthropogenic carbon cycle. Innovative technological solutions and the assessment of their ecological, economic, and social impact are required urgently to validate and exploit the potential of this essential part of future energy systems.

In response to these research needs, **The Integrated Fuel & Chemical Science Center (FSC²)** will address challenges and explore opportunities of the emerging renewable energy-chemistry nexus from the molecules to the system level. The integral rather than competitive analysis of feedstocks from atmospheric, biogenic, and industrial sources will lead to a comprehensive design framework for “bio-hybrid fuels and chemicals”.

3.2 Vision and Mission



The Integrated Fuel & Chemical Science Center generates fundamental knowledge and novel scientific methods for the development of adaptive technical solutions to valorize renewable electricity and feedstocks into liquid energy carriers and chemicals in a systems approach.

Figure 1: Vision and Mission of The Integrated Fuel & Chemical Science Center (FSC²)

Within The Integrated Fuel & Chemical Science Center (FSC²), RWTH Aachen University (RWTH) and its strategic partners Forschungszentrum Jülich (FZJ) and Max Planck Institute for Chemical Energy Conversion (MPI CEC) take an integrated approach embracing natural sciences, engineering sciences, and social and economic sciences to encompass their complementary competencies on the molecular, device, and systems level to understand, master, and design sustainable processes for harnessing renewable energy in liquid energy carriers and chemicals. FSC² will provide a science-driven framework for structural developments between RWTH, the FZJ of the Helmholtz-Association and the MPI CEC in the Max-Planck-Society. This includes agreements for open access to infrastructures as well as joint appointments for junior and senior researchers. It therefore integrates synergistically three different major institutions of the research and education system in Germany.

FSC² has its roots in the Cluster of Excellence (CoE) The Fuel Science Center (FSC). A unique interdisciplinary research culture was established overcoming disciplinary boundaries through composing the extended expertise of the research network in interdisciplinary Competence Areas (CAs) according to the time- and length-scales of the molecular, device, and systems level. Focusing initially on the intricate relationship of combustion properties and the molecular struc-

ture of carbon-based fuels as common denominator, a “fuel design process” was successfully established for the first time. A substantial number of high-level publications from interdisciplinary and interinstitutional teams showcases the collaborative spirit as basis to enter into uncharted scientific territory. During this development, the synergistic potential of the studied production technologies for energy carriers as well as chemical products became increasingly obvious as reflected by life cycle assessment and socio-economic analyses. This background places the partner institutions and network of Principal Investigators (PIs) now in a unique position to align groundbreaking science on the [production of fuels and chemicals with focal technology options for molecule-based energy conversion systems in light of systems analysis](#). To express the [Fundamental Science](#) approach embracing [Systems level analysis for Fuels and Chemicals](#) within an integrated research [Center](#), we have chosen [FSC²](#) as acronym, illustrating simultaneously the successful branding and the adaptivity of the research framework to new directions.

Based on the previous scientific and structural achievements (see Chapter 4.2 and 4.3), [FSC²](#) is able to respond to the dynamics in the global energy system by expanding and refocusing its research program into novel areas. We propose to carry the unique interdisciplinary approach to a next level by (i) expanding the systematic bio-hybrid design process to integrate fuel and chemical production explicitly, (ii) addressing nitrogen-based substances and in particular ammonia newly in the integrated fuel and chemical design process, (iii) extending the technologies for fuel conversion by considering their applicability to existing vehicles as well as energy conversion in fuel cells for future propulsion systems, (iv) integrating innovations in individual catalysis disciplines strategically in optimized process chains, and (v) intensifying the development and use of digitalized research data management and machine learning methods. In particular, [FSC²](#) will address the following key questions originating from the vision and mission outlined above:

- How can global energy and material cycles be made [adaptive and resilient](#), while fulfilling all three dimensions of sustainability – [ecological, economic, and social](#)? Current research often focuses on individual aspects of fuel and chemical conversion systems, e.g., individual levels of the system, or certain aspects of sustainability. Moreover, disruptions to the systems’ supply and operation are often neglected, and the dynamics of the ongoing long-term transformation towards climate-neutrality are not sufficiently covered. Therefore, there is a need for an integrated approach to design and operate these systems to be resistant to withstand and resilient to quickly recover from disruptions, and to be adaptive to adjust to variability in supply and demand and long-term transformation processes. The approach must encompass all dimensions of sustainability at every level, from individual processes to the broader supply chain and system level.
- How can [translational catalytic processes](#) at the direct interface of energy and feedstocks be designed to cope with the dynamics and variations of their supply? In current catalysis research on renewable carbon feedstocks, there is a strong focus on developing novel transformations often using simple and pure model compounds. However, an envisaged process

3 Objectives of the Cluster of Excellence

requires the additional fulfilment of certain catalyst performance criteria in terms of activity, selectivity, and stability when dealing with real starting materials. Solvents and reactants characteristics need to be integrated with downstream processing and product isolation to achieve minimal energy use and environmental footprint.

- How can chemical, biochemical, and electrochemical transformations for the manipulation of C – H, C – C, C – O and C – N bonds be interlinked to open **concatenated synthetic pathways** to fuels and chemicals? The transformations of bio-based, CO₂-based and nitrogen-based building blocks are usually addressed by the individual catalysis disciplines of molecular, heterogeneous, electro-, or bio-catalysis. To establish effective connections between starting materials and desired molecular architectures, however, the transformation steps need to be designed and developed with a focus on the transfer points of intermediate products, reaction media and the recycling of the catalyst system from the beginning. Therefore, the selection of the most appropriate catalytic discipline is not determined solely by the evaluation of the individual catalytic transformation, but rather by the most efficient contribution within a transformation cascade of concatenated catalytic steps.
- How does the molecular structure of **carbon-based fuels** impact efficiency and emissions upon recuperation of the chemically stored energy in fleet-compatible thermal or future electrical propulsion systems? In the current phase, all degrees of freedom of bio-hybrid fuel molecules and molecularly controlled combustion systems were exploited to achieve the highest possible efficiency with near-to-zero pollutant emissions. The task now is to transfer this knowledge to the optimization of propulsion systems under the tight constraints regarding possible modifications, due to the demand of applicability to existing vehicles. Research into electrochemical energy conversion is currently focused almost exclusively on hydrogen as an energy carrier. Here, the potential of direct liquid fuel cells is now to be unlocked through the integrated fuel design process.
- How can engines and devices be designed to exploit **ammonia as fuel** most effectively? Ammonia's low reactivity and its tendency to form oxides of nitrogen pose major challenges to achieving high energetic efficiency and low emissions in thermochemical utilization. Solutions will be developed combining the molecular-torch concept with utilizing partial in-process reforming to hydrogen and innovations in exhaust gas aftertreatment specifically for the very potent greenhouse gas N₂O.

3.3 Objectives

Based on the vision as well as resulting scientific challenges and key questions, FSC² defines its scientific and structural objectives (see Table 3.3).

Table 3.3.1: Objectives of The Integrated Fuel & Chemical Science Center

Scientific Objectives
Enable optimal overall efficiency, from co-production of chemicals and fuels <i>via</i> common intermediates to propulsion in existing and novel propulsion technologies; this is done by developing and combining cutting-edge methods from molecular design, propulsion equipment design, production process development, and machine learning.
Design sustainable pathways from renewable energy and carbon resources, nitrogen and hydrogen to chemical and energy intermediates eventually allowing the synergistic production of bio-hybrid fuels and chemicals.
Enable concatenated bio-, chemo- and electro-catalytic transformations for bio-hybrid fuels and chemicals by integrated catalyst, reactor and process development, complemented by the tailored interplay with modeling approaches, ultimately leading to the establishment of digital tools for the predictive catalyst-process design and their validation in view of feedstock variation and energy fluctuation in post-fossil value chains (translation).
Enable beyond 50 % energy conversion efficiencies and near-zero pollutant emissions by developing bio-hybrid-fuels based on novel and fleet-compatible engine concepts with advanced molecularly-controlled combustion and aftertreatment technologies.
Exploit the potential of novel carbon- and ammonia-based fuel cell concepts as well as ammonia-fueled combustion engines based on the fundamental understanding of the involved thermochemical and electrochemical processes.
Design resilient and sustainable global conversion systems that integrate FSC ² pathways, fuels, and chemicals with competing and synergistic pathways and products, taking into account systemic risks, stakeholder perspectives, policies, and sustainability criteria.
Structural Objectives
Furnish a world-class research environment through the convergence of disciplinary research and strategic collaboration of RWTH with the Max Planck Institute for Chemical Energy Conversion and the Helmholtz-Center Jülich. Thus, FSC ² will generate prolific and highest quality scientific output including joint publications, enable the individual researchers to take a leading role in the scientific community, and provide a stimulating framework for translational research.
Strategic development of FSC ² through 12 appointments of tenure track and lighthouse professorships in inter-faculty and inter-institutional frameworks; this will strengthen the core competences as well as new strategic research areas, particularly in the field of digital chemistry and fuel cells beyond hydrogen.
Accelerated talent development of early career researchers; this will be accomplished through a comprehensive set of developmental measures and an individualized curriculum organized within FSC ² Research School, including the installation of 5 Junior Research Groups.
Foster an inclusive and diverse research culture with the aim to increase the diversity within the team across disciplines and hierarchies of FSC ² by establishing a tailor-made research-oriented diversity approach. This includes a diversity survey based on various diversity categories (e.g., gender, national background, family duties) enabling an intersectional diversity perspective to gain insights in challenges and opportunities of the team structure, according to the needs formulated by the members of the cluster.

4 Research Program

4.1 Research Objectives, Research Approach, and Positioning Within the Research Area

4.1.1 Objectives and Approach

The Integrated Fuel & Chemical Science Center (FSC²) uses a systems approach to generate fundamental knowledge and novel scientific methods for adaptive technical solutions that valorize renewable electricity and feedstocks into chemical energy carriers and products. Scientific competences covering the molecular, device, and systems levels and their interdisciplinary connections enable fundamental research towards (i) thermal and electrochemical energy conversion processes using carbon- and ammonia-based energy carriers, (ii) chemo-, bio-, and electro-catalytic synthesis and production processes for fuels and chemicals, and (iii) an integrated design approach of conversion systems for sustainability and resilience on a global scale.

FSC² will continue the successful development and application of a broad range of methods: e.g., from multiphysics modeling of devices to multiscale optimization of value chains; e.g., from quantum mechanics to synthesis of adaptive catalysts. The importance of machine learning techniques will continue to substantially grow, e.g., for the prediction of fuel properties or catalyst performance. The overarching research objectives of FSC² are summarized in Table 3.3. The highly interdisciplinary research activities are allocated within five Strategic Research Areas (SRAs) in the research structure described in Section 4.3 and discussed in detail in Section 4.5.

The scientific approach is outlined briefly here.

Two SRAs focus on **energy conversion systems** using molecular energy carriers with particular **emphasis on difficult to electrify propulsion systems** for on-road and marine mobility and transportation. In the SRA “Carbon-based Fuel Application” (SRA-CFA), the fuel design process successfully established in the previous phase of The Fuel Science Center (FSC) will be developed further in a focused direction taking into account new boundary conditions from expected constraints in future engine development. In the SRA “Ammonia Fuel Utilization” (SRA-AFU), the direct use of ammonia as energy carrier will be

studied as complementary strategy to harness renewable energy for sustainable propulsion. In both SRAs, thermal energy conversion through combustion as well as electrochemical conversion in fuel cells will be envisaged focusing on thermodynamic efficiency, emission analysis and control, engine components, and systems integration.

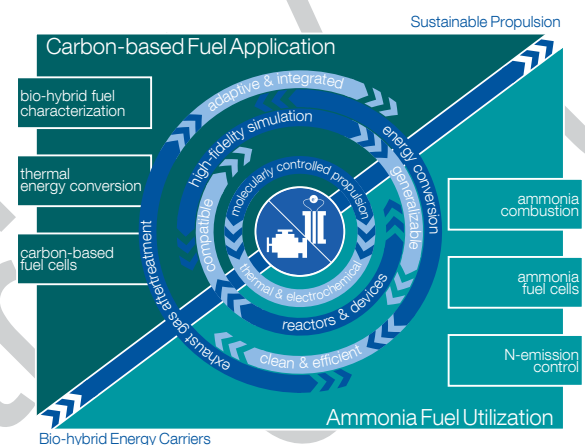


Figure 2: Methodologies and targets of SRA “Carbon-based Fuel Application” (SRA-CFA) and SRA “Ammonia Fuel Utilization” (SRA-AFU)

4.1 Research Objectives, Research Approach, and Positioning Within the Research Area

Two SRAs focus on **production processes** using non-fossil feedstocks and energy from renewable sources for the synthesis of **bio-hybrid fuels and chemicals**. In the SRA “Concatenated Synthetic Pathways” (SRA-CSP), innovative methods based on chemo-, bio- and electro-catalytic transformations will be explored for the selective formation of C-H, C-C, C-O, and C-N bonds with the aim to integrate the individual transformations into optimized synthetic pathways (concatenation). Carbon dioxide and platform chemicals derived from lignocellulosic biomass will constitute the main carbon building blocks, and ammonia or simple derivatives thereof are envisaged as nitrogen building blocks. Hydrogen or electrons will provide the “green” redox equivalents to achieve the necessary molecular manipulations. In the SRA “Translational Catalytic Processes” (SRA-TCP), the new reaction types and pathways will be validated in view of challenges related to feedstock variation and energy fluctuation in realistic post-fossil production systems (translation). Similar to the two SRAs on propulsion systems, the two SRAs in production share certain common experimental techniques and modeling and simulation methods creating a synergistic toolbox.

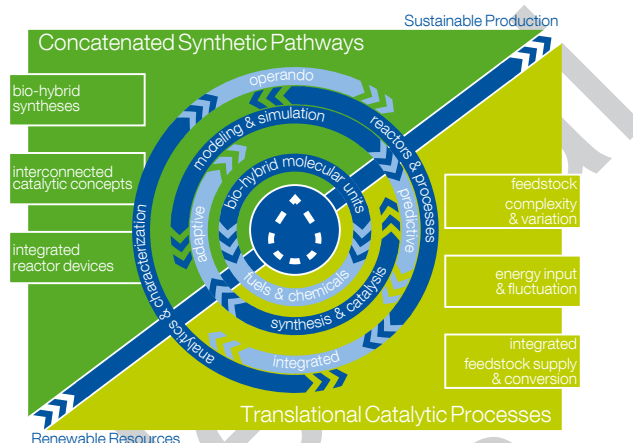


Figure 3: Methodologies and targets of SRA “Concatenated Synthetic Pathways” (SRA-CSP) and SRA “Translational Catalytic Processes” (SRA-TCP)

In SRA “Resilient & Adaptive Conversion Systems” (SRA-RACS), an integrated & interdisciplinary systems approach is used for the design & operation of resilient & adaptive conversion systems accounting for all dimensions of sustainability. In order to meet its scientific and technical objectives, FSC² will need to push methodological boundaries in all three competence areas. The approach will encompass all dimensions of sustainability, economic, social and environmental. Model-based optimization-assisted methods will be coordinated across the cluster in a problem-oriented research team ensuring knowledge transfer and synergy among the different groups and covering all levels, from the product, to devices & processes, to the broader supply chain and system level. The SRA is structured around fuel & chemical design, system integration and sustainability assessment. The results of SRA-RACS are fed back to the other SRAs consistently to enable an iterative research process within FSC² based on an ex-ante evaluation of developed process paths and fuels.

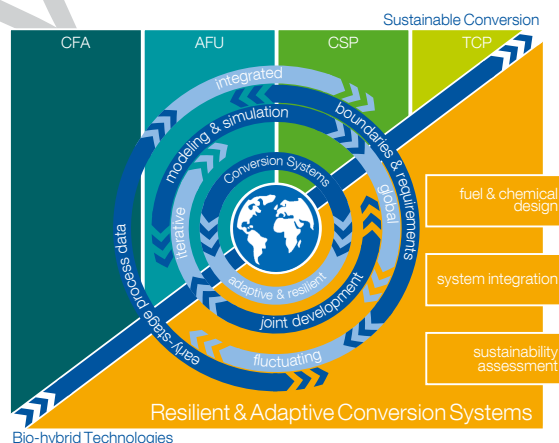


Figure 4: methodologies and targets of SRA “Resilient & Adaptive Conversion Systems” (SRA-RACS)

Working groups will be formed for common topics and techniques with the potential to cross-

4 Research Program

fertilize the progress of the SRAs. This includes for example machine learning, methods for the preparation and characterization of materials, the integration of production pathways and propulsion properties, and the seemingly contradicting goals of integration for process chains and flexibility of individual process steps.

4.1.2 Position of FSC² within the National and International Research Area

The so far established FSC in its broadness to cover fuel production and propulsion in an integrated approach has been unique. The Co-Optima program by the US Department of Energy (DOE) as one of the very few large-scale initiatives embracing fuel production and propulsion has ended in 2022. Existing academic-industrial networks such as the Kopernikus projects “Power-to-X” and the BMBF initiative “Carbon2Chem®” are rather translational than fundamental. In its new extension to chemicals, FSC² as a strategic partnership between RWTH and its Partners FZJ and MPI is a unique initiative in its fundamental and broad character, providing an excellent infrastructure and a critical mass of leading scientists, capitalizing on the individual profiles of the institutions within the German scientific landscape. Through our scientific and industrial advisory board, we will ensure a constant monitoring regarding existing and upcoming initiatives and seek cooperation with research institutions as well as industry at an earliest possible stage.

4.2 Preliminary and previous work

The Cluster of Excellence (CoE) FSC has established a unique and world-leading research platform for the design of liquid energy carriers for CO₂-neutral and near-to-zero pollutant emission propulsion systems. The research went far beyond conventional approaches by defining the scientific basis for the development of bio-hybrid fuels, integrating renewable electricity with the co-use of bio-based carbon feedstocks and CO₂. Fostered by interdisciplinary collaboration from the molecular level through the modeling and demonstration of advanced devices to multifactorial systems analysis, adaptive production and propulsion technologies have been developed under dynamic system boundaries. Temporary translational research teams have enabled insights from basic research to be integrated into the various research areas, thus supporting the elaboration of specific new technologies in fuel science. With the comprehensive implementation of the objectives defined in FSC, the way has now been paved to address the next level of complexity at the energy-chemistry nexus by Fundamental Science embracing Systems thinking for Fuels and Chemicals within an integrated Center structure in FSC².

A central objective of the interdisciplinary collaboration in FSC was to identify promising target structures for sustainable fuels in the Fuel Design Forum (FDF) and to integrate their production path with the performance of the propulsion system [1]. Maximizing carbon efficiency and minimizing energy consumption are essential design criteria for the production processes of bio-hybrid molecules that unlock the synergistic potential of biomass and CO₂ feedstocks. The integration of innovative bio-, chemo-, and electrocatalytic methods for catalytic CO₂ conversion with biomass-derived building blocks opened unprecedented synthetic routes to fuel targets be-

yond established products. Finally, the potential of these new bio-hybrid fuels, when combined with modern engine designs and technologies, to increase efficiency while reducing emissions has been demonstrated [2].

Examples illustrating the interdisciplinary approach include the preparation of structurally versatile cyclic acetal bio-hybrid fuels by integrating bio-catalytic alcohol formation and chemocatalytic CO₂ utilization, ultimately leading to a tailored apparatus for sequential product formation and purification with minimal energy consumption. The adaptive synthesis route enabled systematic structural variation of the bio-based component and detailed investigations of structure-performance relationships in established and advanced engine technologies, thereby gaining unprecedented insights into combustion mechanisms [3]. In particular, engine concepts that rely on the combined use of low- and high-reactivity fuels (molecular torch (MT) and molecular spark (MS)) have been shown to achieve ultra-high thermal efficiencies of up to 49%. Furthermore, FSC was able to develop hydroformylated Fischer-Tropsch fuels (HyFiT) by covering all aspects from catalytic production to combustion properties and material compatibility to systems analysis. Thus, HyFiT fuel production closes the carbon cycle in a flexible way by using either biomass or carbon dioxide as feedstock, while being scalable through mature technologies. Finally, vehicle tests showed a significant reduction in particulate matter and nitrogen oxides caused by combustion [4].

The detailed insights gained from such iterative studies were combined with advances in modeling and simulation as a basis for mathematical optimization methods across all levels. This was successfully demonstrated for the holistic development of a bio-hybrid fuel blend made of four different components. Using the process network flux analysis (PNFA) developed within the FSC, a blend with optimal CO₂ reduction, costs, and life-cycle assessment (LCA) indicators such as land use was determined. Challenges and opportunities arising from the use of electricity from renewable sources as the primary energy input for the production processes were addressed by strategically integrating electrocatalysis already on a molecular and device level [5].

In summary, the unique FSC approach enabled the development of adaptive production and propulsion technologies across all length scales through cross- and interdisciplinary collaboration. The results summarized here are presented in more detail in Chapter 4.5.

FSC's adaptive structure has been successfully used to integrate associated PIs at different career stages and to ensure an effective mix of continuity and rejuvenation of a diverse research team at all levels. The seamless integration of strategically planned appointments at various faculties and institutions demonstrates the pronounced structural effect of the cluster. The benefit for scientific progress was a key driving force for unprecedented forms of structural cooperation between RWTH Aachen University, the Forschungszentrum Jülich, the Max Planck Institute for Chemical Energy Conversion and the Max Planck Institute for Coal Research. The resulting tailor-made network was instrumental in establishing several important large-scale collaborative projects with strong translational components (ReDiFuel, catalaix, Helmholtz-Cluster Wasserstoff HCH₂, Kopernikus Power-to-X, Carbon2Chem, NaMoSyn).

4 Research Program

Consequently, the goal-oriented, successful demonstration of individual scientific excellence, interdisciplinary team spirit and institutional collaboration in the FSC provides a solid basis for the generation of fundamental knowledge and methodological know-how in the FSC².

4.3 Structure of the research program

The concept of interdisciplinary Competence Areas (CAs) and their effective and dynamic interconnection, successfully established in the current FSC, now form the backbone of the **unique research framework of FSC²** allowing the cluster to flexibly address the challenges resulting from the “defossilization” of energy carriers and chemicals. The central achievement of the Competence Areas (CAs) is the convergence of expertise from various disciplines along the length and time scales of the overall system levels: (CA1) Molecular Transformations and Interactions, (CA2) Interfacial Phenomena and Devices, (CA3) Fuel Design and Sustainable Cross-sectorial Value Chains.

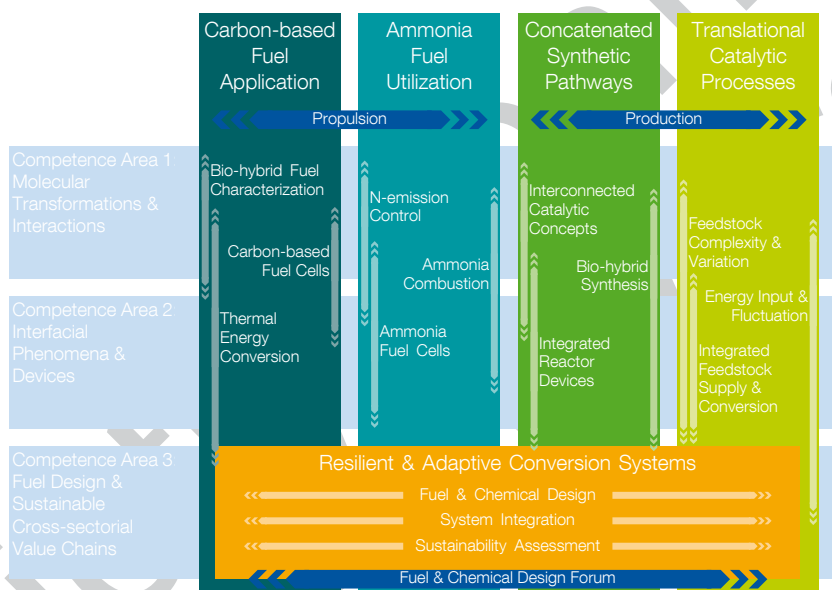


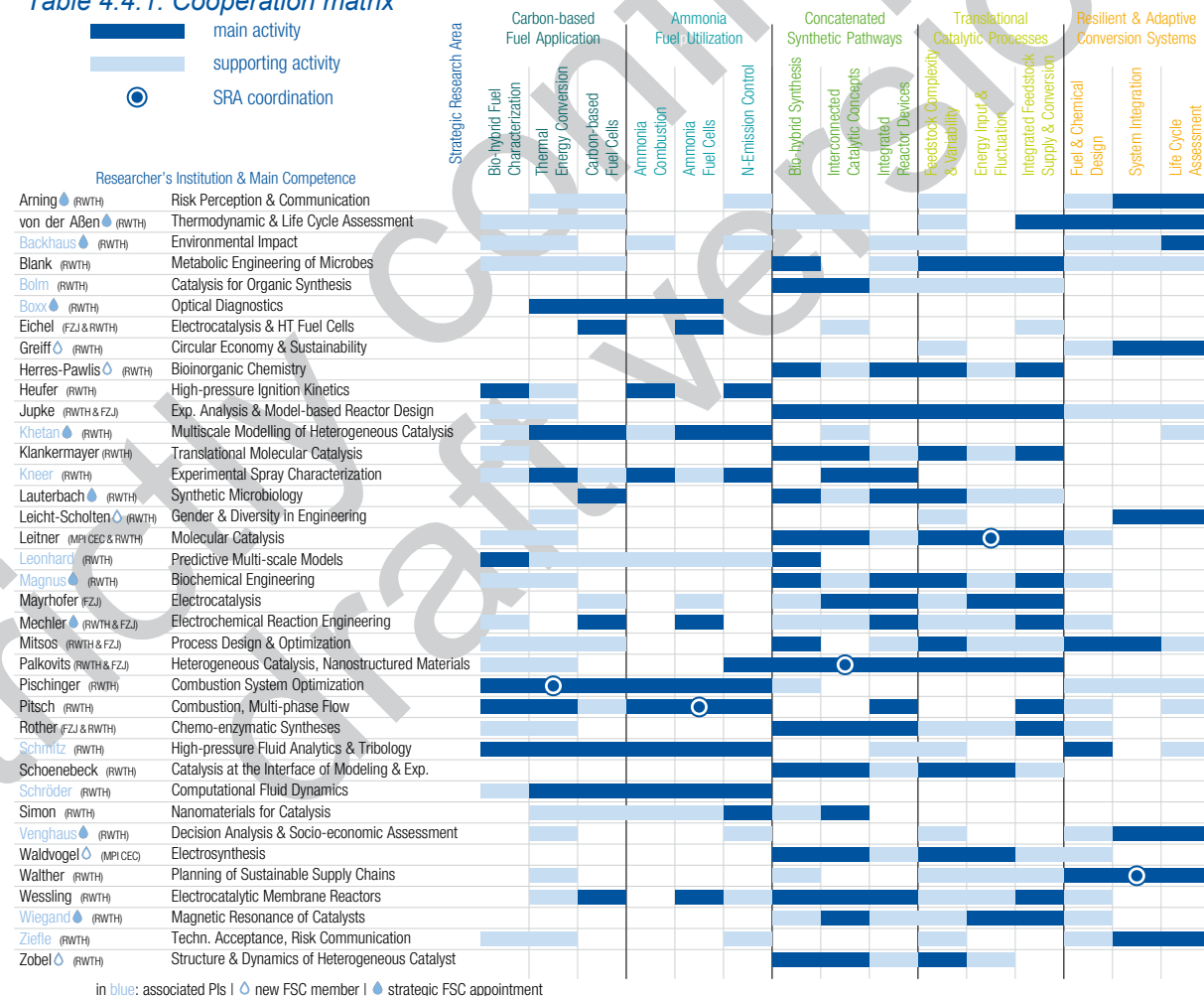
Figure 5: The integrated framework of the five Strategic Research Areas (SRAs) embedded within the Competence Areas (CAs).

Moving forward, all research activities and projects are allocated within the five SRAs, which encompass and simultaneously stimulate the disciplinary progress of the individual PIs, thus constantly augmenting the CAs (Figure 5). The SRAs are bridged via general design challenges that will be addressed in flexible working groups as the research program develops. This includes the integration of production pathways and propulsion properties for the carbon-based fuel design and the exploration of fundamental mechanisms of electrochemical ammonia activation for energy or synthetic applications. Another design challenge at system level involves reconciling the integration of process chains with the simultaneous flexibility of individual process steps. On top of that, the interdisciplinary exchange across all SRAs will be taking place in the Fuel & Chemical Design Forum (FCDF).

4.4 Staff and institutional composition of the Cluster of Excellence

The three CAs are represented by 25 core Principal Investigators (PIs) who define the thematic focus within the SRAs. However, the work of the cluster is based on a much larger network of scientific excellence and methodological expertise through 12 associated PIs. All PIs have the same rights and responsibilities within the cluster, creating the necessary critical mass and structural impact among the three partner institutions RWTH Aachen University (RWTH), Forschungszentrum Jülich (FZJ) and Max Planck Institute for Chemical Energy Conversion (MPI CEC). During the current phase, new research fields and emerging areas as well as four core research areas have been strengthened by integrating four new researchers from RWTH and one from MPI CEC to the network of PIs within FSC (◊) and by 10 FSC-oriented strategic appointments (◆) at the partner institutions. The main areas of competence of the individual PIs and their contribution to the research program are summarized in Table 4.4.1.

Table 4.4.1: Cooperation matrix



Based on various multilateral previous collaborations, the partners will form a tightly knit collaborative and interdisciplinary scientific environment combining a unique set of expertise. Most PIs have participated in or even coordinated collaborative research centers and research training groups funded by the DFG or large-scale projects on national or European level (for details see

Section 6.3 and individual CVs). The PIs have state-of-the-art research facilities and cutting-edge equipment at their disposal to host the FSC² activities in a strategically coordinated virtual center creating synergies across the institutions. A particular strength of the consortium in this context results from the fact that several PIs share dual appointments between the collaborating institutions (RWTH/FZJ: Eichel, Jupke, Mechler, Mitsos, Palkovits, Rother; RWTH/MPI CEC: Leitner, Palkovits, Wiegand).

The PIs are renowned experts in their fields as evidenced by their publication records and other relevant criteria of the respective scientific disciplines. Individual recognitions include a Leibniz Prize, the "Project of the Century" Research-Award from the Werner Siemens-Foundation, a Humboldt professorship as well as a Heisenberg Professorship, five ERC grants (three advanced, two starting), and several further prestigious national and international awards (for details see Appendix A.3 and individual CVs). The international reputation of the team is further reflected by the commitment of leading scientists and industrial stakeholders to support and critically accompany the cluster activities in the International Advisory Board (see Table 5.4.1). In FSC², the recruitment of 13 new faculty members as listed in Table 6.2.1 (Section 6.2) including new appointments, as well as early-succession models, will ensure the continuous rejuvenation and diversity of the network of PIs, enriching the cluster with complementary knowledge and methods. The PIs cover all academic career stages as basis for the longterm development of the research area. The FSC² foresees the integration of further associated researchers depending on the temporary formation of translational projects with flexible fund allocation. This adaptive approach results in a CoE structure with a stable core allowing at the same time for flexibility where required.

The collocation of the PIs and their expertise is particularly well suited for tackling the challenges to be addressed in the FSC². In SRA-CFA and SRA-AFU, a detailed understanding of the phenomena relevant for the molecularly controlled propulsion systems including combustion as well as electrochemical energy conversion and advanced aftertreatment is mandatory. This is covered by the researchers' expertise in fuel injection, spray and mixture formation, in-cylinder fluid dynamic and combustion process (Kneer, Schröder, Pitsch, Pischinger) combined with competences in methodological laser spectroscopy (Boxx) and in tribology and hydrodynamics (Schmitz). The molecular basis of combustion will be covered through expertise in experimental methods for autoignition chemistry and pollutant formation as well as chemical kinetic modeling and chemistry reduction (Pitsch, Heufer), adding competence in quantum chemistry and molecular dynamics (Leonhard). Dealing with the aftertreatment systems and catalytic surface coatings in the combustion chamber requires a combination of expertise in catalytically active materials (Palkovits, Simon), multiscale modelling of heterogeneous catalysis (Khetan), as well as an integrated catalyst system layout in the context with the engine requirements (Pischinger, Heufer, Wessling). The new research topic of electrochemical energy conversion of liquid energy sources and ammonia in fuel cells is being investigated in a holistic approach starting from the electrochemical fundamentals (Eichel, Mayrhofer, Palkovits, Lauterbach) *via* the process level (Mechler, Mitsos, Wessling) to system integration (Pischinger).

Numerical and experimental evaluation of multiphase reactive flow (Schröder, Khetan) leads to a detailed understanding of the underlying electrochemical processes.

The exploration of different production pathways is addressed in SRA-CSP and SRA-TCP. The expertise of the responsible PIs in the field of catalysis cover competences in heterogeneous catalysis (Palkovits), homogeneous catalysis (Bolm, Herres-Pawlis, Klankermayer, Leitner, Schoenebeck), and biocatalysis (Blank, Lauterbach, Rother). Of note here is the established integration and exchange with PIs in the research area of electrochemistry (Eichel, Mayrhofer, Waldvogel). The network is further extended by experts in extensive analytics such as liquid and solid-state NMR or X-ray absorption and emission spectroscopy (Wiegand, Zobel). To bring the identified pathways from lab-scale to a technical scale and to combine them into overall processes, fundamental design aspects of production steps and processes are being investigated and addressed by PIs with expertise in reaction and process engineering of (bio-)catalytic transformations (von der Aßen, Jupke, Leitner, Magnus, Mitsos, Wessling) as well as electrochemical devices (Eichel, Mechler, Wessling).

The SRA-RACS aims to develop a predictive and holistic approach for the design of fuels and chemicals. To this end, researchers provide expertise in predictive models linking molecular structures to performance of liquid energy carriers and chemical building blocks (von der Aßen, Mitsos, Pischinger, Pitsch). The network of PIs cover competences in models depicting the coupling of the sectors energy, transport and chemistry (von der Aßen, Walther). These models are extended by socio-economic and socio-political implications, specifically regarding aspects of systemic risk analysis (Arning, Ziefle), stakeholder incentives (Walther, Venghaus), and policy design (Venghaus, Walther). The results are combined with a sustainability assessment (von der Aßen, Backhaus, Greiff, Leicht-Scholten) in an iterative design cycle to achieve resilient and adaptive fuel and chemical conversion systems.

In addition to the excellent global network of each individual PI, strategic collaborations with international centers of excellence in closely related activities, such as the Future Energy Systems (FES) program at the University of Alberta, the recently established research program Renewable Fuels and Chemicals for Switzerland (refuel.ch) in the ETH domain and the Japanese Decarbonized Industrial Thermo-System Center (DITS), are being promoted and established as part of the FSC activities (see section 6.3).

To ensure an unbiased reflection on the results, the Cluster of Excellence (CoE) calls on the independent expertise from the Institut für Energie- und Umweltforschung Heidelberg gGmbH (ifeu). In this context, critical assessments for specific case studies are commissioned and their experts are invited to participate in the Fuel and Chemical Design Forum. This approach provides important feedback for the continuous structuring progress of the research activities and allows to benchmark the technological perspectives resulting from the fundamental research within FSC² with other developments in a dynamically changing energy and mobility landscape. The dissemination of the research results and public outreach will be supported by the state agency for energy and climate protection in North Rhine-Westphalia (NRW.Energy4Climate), e.g. by organizing workshops with scientific and non-scientific stakeholders.

4 Research Program

4.5 Detailed Description of the Research Program

4.5.1 SRA "Carbon-based Fuel Application" (SRA-CFA)

PIs: [Pischinger](#), Blank, Eichel, Heufer, Klankermayer, Lauterbach, Leitner, Mechler, Mitsos, Palkovits, Pitsch; ARs: Boxx, Kneer, Leonhard, Schmitz, Schröder, Simon

The SRA-CFA focuses on the conversion of carbon-based fuels in existing and future propulsion systems, including both internal combustion engines (ICEs) and fuel cells. High efficiencies and near-to-zero pollutant emissions were achieved in FSC using novel bio-hybrid fuels and fundamentally new combustion systems like molecularly controlled combustion systems (MCCSs), which required dedicated engine designs [6, 7]. However, current propulsion systems will continue to have a significant share of the vehicle fleet in the decades to come [231, 234]. Hence, there is a high motivation to design fuels and novel combustion systems which can be implemented into existing vehicles, so-called retrofit solutions. Such retrofit solutions are subject to adaptivity constraints that might limit the potential efficiency increase and emission reduction. For instance, a compression ratio (CR) increase would be limited to an adaptation of the piston, since an increase of the stroke is not feasible. The resulting increased surface-to-volume ratio will lead to increases of both the wall heat transfer and the hydrocarbon emissions, leading to reductions of the efficiency. Therefore, we will build-up on the methodologies that we developed in FSC and extend them to the fuel candidates under adjusted boundary conditions. As new carbon-based fuels become available, it will also be attractive to apply them in direct liquid fuel cells (DLFCs). The fuel design process will be extended to DLFCs to exploit the potential of a co-optimization of the fuel and the DLFCs, taking into account the limitations regarding efficiency and durability of current state-of-art low and high temperature DLFCs.

Strategy and Structure of SRA

The SRA-CFA explores the efficient conversion of liquid energy carriers in form of hydrocarbon molecules, focusing on **bio-hybrid fuels and fuel blends**. The research topics include the **combustion processes** and the **electrochemical conversion** on the molecular level (CA1) as well as the associated energy conversion systems **ICEs** and **DLFCs** on the device level (CA2). In line with the holistic, integrated **Fuel & Chemical Design Process (FCDP)**, the results contribute (i) to defining requirements for new fuel molecules and blends (SRA-TCP & SRA-CSP) and (ii) to the design and assessment of resilient and adaptive mobility systems (SRA-RACS).

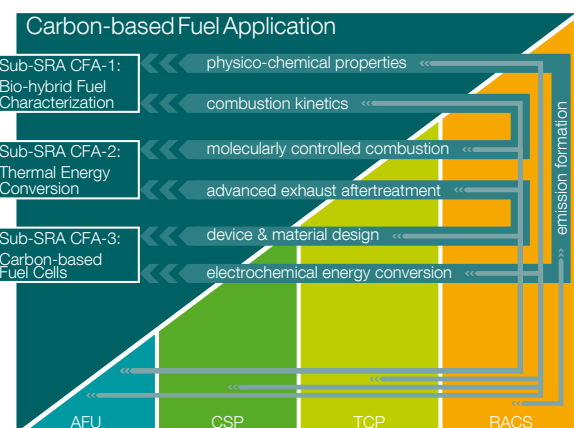


Figure 6: Structure of the SRA-CFA

FSC² transfers the findings on MCCSs as well as on high-performance and high-adaptivity

aftertreatment systems in combination with bio-hybrid fuels to **molecularly controlled propulsion systems (MCPSs)**, introducing the concept of **fleet-compatible fuel and powertrain co-optimization**. With the new research field of **DLFCs**, electrochemical energy conversion systems are integrated into the **FCDP** to harness their potential for high efficiencies combined with high energy and power densities.

4.5.1.1 Bio-hybrid Fuel Characterization

The focus of the overarching optimization problem within the Fuel & Chemical Design Process has been on minimizing greenhouse gas emissions and the environmental impact of pollutant emissions as well as resource-efficient production. These still essential target variables are now supplemented by the compatibility of the fuels with existing powertrains opening up new research questions regarding the physico-chemical properties and requirements of bio-hybrid fuels and fuel blends in both fleet compatible thermal as well as prospective electrochemical conversion systems. Complex reaction mechanisms and molecular interactions are understood and modeled using machine learning (ML) methods in combination with intelligent sampling techniques and integrated into the established Fuel & Chemical Design Process. The in-depth understanding of the efficient energy conversion, emission formation, and molecular interaction of compatible bio-hybrid fuels is fed back into production (SRA-TCP & SRA-CSP) and contributes to the comprehensive LCA (SRA-RACS) as well as the design of molecularly controlled energy conversion systems.

Current State of Research and Previous Work

Managing complexity is one of the biggest challenges of chemical kinetic development. State-of-the-art, detailed chemical kinetic development requires compiling models with hundreds of species and thousands of reactions, determination of the associated parameters and their uncertainties, and validation of new models against data from numerous sources. Several detailed kinetic models were successfully developed as part of FSC for prediction details of pyrolysis and oxidation behavior of fuels [8–12]. Such developments base on a detailed theoretical calculation of molecular dynamics (MD) [13, 14] [179] with the highly recognized FSC-tool ChemTraYzer (CTY) (reviewed by [235–237]), on high-level quantum mechanics (QM) calculations of rate constants [15, 16], and thermodynamic data [17], as well as experimental results on laminar burning velocity (LBV) [18], ignition delay times (IDTs) [19], species measurements in flow reactors [20], and flame emissions [3, 21] produced within the cluster and through external cooperation.

Though effective and successful, processes established in the FSC show that the involved human efforts remain high. Several tools and methods have been devised in response to this challenge. Within the FSC, model-based experimental design has been used to identify optimal conditions for experimental measurements [22] and a comparative quantitative analysis of ammonia combustion models [23] demonstrated how knowledge of complex oxidation processes can be consolidated. Other popular approaches are automatic model generation [180] [238] and parameter estimation [238].

Recent advances in data-driven ML, particularly in natural language processing (NLP) techniques [239, 240] [24], could unlock new potential for managing complexity, making the kinetic model development process more efficient, reliable, and adaptable to evolving demands.

Universal differential equations (UDE) emerged from a special focus on incorporating fundamental physical principles in ML-based models for dynamical systems allow the combination of theoretical models with data driven training to increase computational efficiency and extrapolation capability [241]. Owoyele and Pal [242] have shown that Neural Ordinary Differential Equations, a sub-type of UDEs, can be used to mimic a classical hydrogen kinetic model at a fraction of the computational cost. Here, the incorporation of prior knowledge was substituted by an iterative training approach, which does not scale well with larger mechanisms. The incorporation of physical constraints like energy- and atom-balance and the flexibility of neural networks as universal approximators to achieve a higher accuracy in combination with a universal global reaction scheme [25] will be key to the further development of this method.

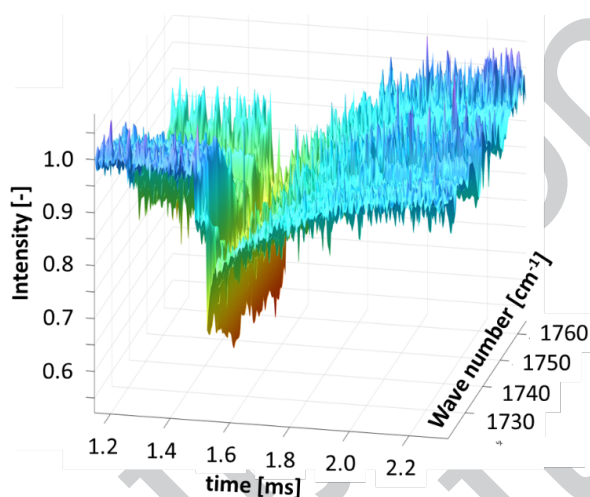


Figure 7: Measured time-resolved IR-absorption spectra during ethylformate pyrolysis

To gain detailed knowledge about the combustion chemistry, particularly emission formation, laser absorption spectroscopy (LAS) and gas chromatography and mass spectrometry (GCMS) are used. LAS is a non-intrusive in-situ method, that directly measures in a shock tube (ST) or rapid compression machine (RCM). Both facilities are already in use to study the combustion of potential bio-hybrid fuel candidates [10–12, 19, 26, 27]. For in-situ species measurements, a dual-comb infrared (IR) laser setup demonstrated its potential by scanning a wavenumber range 60cm^{-1} with a time resolution of $4\mu\text{s}$ [243] [28]. As this system uses a

wavenumber range, different species can be measured simultaneously. This great advantage, however, leads to a more complex analysis, especially when mixtures should be measured, and not all components are known. A first guess about the different species-spectra that superimpose into the one, measured spectrum, can be achieved with the help of multivariate curve resolution (MCR). However, this method very quickly comes to its limits, especially with unknown species.

Objectives

FSC² aims to devise and implement new numerical and experimental methods to determine the reaction network, thermodynamic, and process performance of bio-hybrid fuels that facilitate an ML-assisted Fuel & Chemical Design Process for both fleet compatible thermal and prospective electrochemical conversion systems.

The exploration of UDE and NLP techniques for kinetic model development and the integration of such ML approaches in established tools like CTY shall enable superior accuracy, generalizability, high computational efficiency, discovery of missing reactions, high-quality datasets, and improved parallelized training strategies. Thereby, FSC² provides a new paradigm in kinetic model development and strives for an interdisciplinary combustion data language in ML, following the FAIR principles.

The computational methodologies will be accompanied by precise experimental measurements to provide meaningful insights into the emission formation of bio-hybrid fuels targeting near-to-zero pollutant emission operation. A new analysis tool for complex multi-component spectra using a combination of QM and MCR aided with GCMS species measurements will be developed to extract crucial information of the complex reaction network.

Work Program

For improving the model development process, one major task is the curation of an extensive database, leveraging high-quality data from experiments and existing chemical kinetic models. This curated data will serve as a foundation for model development, where advanced techniques such as NLP, deep learning, and reinforcement learning will be employed in conjunction with cheminformatics techniques (Tanimoto similarity of reaction fingerprints) to refine and expand existing kinetic models.

In this regard, the validation of rate coefficient predictions and reaction networks will be a critical aspect of this research, employing techniques like k-fold cross-validation and theoretical predictions through molecular dynamics simulations (ReaxFF) and high-level ab initio methods (QM). Automated workflows will be developed for the analysis of heterogeneous systems, integrating tools like Tofhd and CTY for surface detection, event characterization, and reaction network analysis. Quantitative statistical measures, including the curve matching score, will be utilized to objectively assess the model performance and the quality of suggested reactions during the model development.

The research will also focus on integrating ML into model development processes. Semiautomatic ML model development will be pursued, generating training data and optimizing Hamiltonians (Machine learning Potentials) for enhanced accuracy. Active learning methodologies will be implemented to improve ML model performance, utilizing error estimators, and high-level calculations to refine models for reaction kinetics. Alternatively, the development of detailed kinetics could potentially be bypassed by combining global reaction schemes and UDEs in a novel ML approach aiming at fast and robust models for accurate prediction of global properties such as energy release or formation of major pollutants in complex simulations of real application problems. Various loss functions ranging from simple absolute error to complex time wrapping functions, adjoint sensitivity methods for efficient computation of the gradient of the loss function, multiple shooting approach for improved parallelization on multiple cores will be integrated into an automated framework.

Any kinetic modeling approach relies on accurate experimental data for training and validation.

4 Research Program

While the measurement of global combustion properties such as IDTs in STs and RCMs are well established, the focus will be on the development of novel species measuring methods to provide detailed information on intermediate species during the fuel conversion process under application relevant conditions. Current limitations in analysis of time-resolved IR spectra will be overcome by developing a novel analysis tool for complex multi-component spectra using a combination of QM and MCR, supported by novel rapid sample extraction techniques and GCMS analysis.

4.5.1.2 Thermal Energy Conversion

The highly adaptive MCPs are developed along a multi-stage efficiency walk to exploit the potentials of bio-hybrid fuels for the maximum efficiency and the lowest pollutant emissions by considering soft- and hardware modifications to the engines and the exhaust gas aftertreatment systems. The hardware modifications are limited by the applicability to existing vehicles. For instance, an increase of the CR by piston modification causes an increased surface-to-volume ratio, leading to higher wall heat transfer and unburned hydrocarbon emissions. Hence, the near-wall effects will play a decisive role that forms a connection to the SRA-AFU, in which the near-wall effects are crucial due to the slow burning velocity of ammonia. Additionally, close links to the SRA-AFU and to DLFCs exist for both the material compatibility and the exhaust gas aftertreatment. In the FCDP, the propulsion system design is inherently coupled to the LCA. For fleet compatible fuels as well as for the co-optimization of the engine and the exhaust gas aftertreatment, the simultaneous evaluation of fuel candidates and emission legislations as well as the social acceptance play a particularly important role (SRA-RACS).

Current State of Research and Previous Work

In FSC, MCCSs were introduced as the core combustion concepts and investigated on thermodynamic ICEs, supported by fundamental experimental and numerical investigations. Based on the main charge motion, the MCCSs were divided into a high-tumble (HT) approach featuring a molecular torch (MT) and a high-swirl (HS) one using a molecular spark (MS). The MT used an active pre-chamber (PC) application. Here, the main chamber (MC) of the ICE was fueled with a low reactivity (LR) fuel, whereas the PC was fueled with either an LR or a high reactivity (HR) fuel, only requiring a spark plug in case of the LR PC fuel. For the MS, an LR and an HR fuel were directly injected into an ICE with an undivided combustion chamber, controlling the combustion process by the reactivity share and the injection timings of the fuels. The continuous development of the MCCSs yielded a maximum of $\eta_i = 49.1\%$ using $CR = 19$ (Figure 8a) [5–7, 29–33]. For comparison, when using an active PC with gasoline and $CR = 14$, a maximum brake thermal efficiency of 42% was achieved [244], which is a proper value for current series ICEs. The engine-out emissions, especially the NO_x -soot trade-off, were reduced when using the MCCS, representing near-to-zero pollutant emissions (Figure 8b) [7].

On constant volume chambers (CVCs), optical investigations of the penetration length, the spray cone angle, and the liquid fuel probability did not indicate disadvantages of novel bio-hybrid fuels

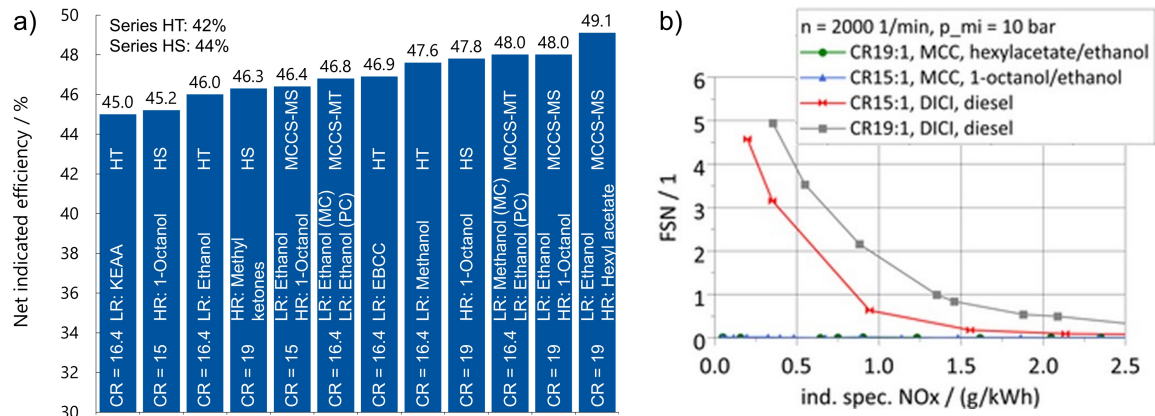


Figure 8: Molecularly controlled combustion systems: a) efficiency walk; b) NO_x-soot trade-off.

over conventional fuels. In addition, the CVC experiments revealed the local formation of combustion products such as CO during the ignition of LR-HR fuel combinations [34]. The charge motion and the mixture formation were investigated on an optically accessible ICE and in numerical simulations, which provided a basis for optimizing the injection timing in the MCCSs [35]. For the MT, numerical ICE simulations and optical RCM investigations revealed the timing of the PC jet ejection into and the ignition locations of the MC charge (Figure 9) [6, 36]. For the

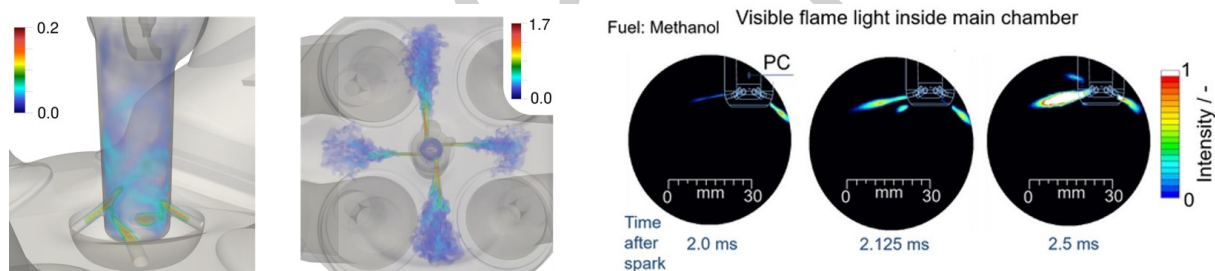


Figure 9: Numerical (left) [6] and optical (right) [36] investigation of pre-chamber jet ejection of the molecular torch.

flame quenching at the combustion chamber walls, a methodology was developed to examine the resulting quench distance in optical RCM investigations using a dedicated quenching object. When using coated quenching objects, the quench distance was reduced [24]. Dedicated exhaust gas aftertreatment systems using microwaves (MWs) to decrease the light-off temperature of catalytic converters revealed that the catalysts performance depended not only on the thermal MW input and composition (i.e. the degree of substitution in the oxide lattice) but also on the specifics of an MW-based activation treatment [37]. The MCCS-related investigations were not only performed for novel neat bio-hybrid fuels but also for fuel blends. The highly knock-resistant blend EBCC¹ slightly outperformed ethanol, whereas KEAA² achieved a similar η_i to 2-butanone, see Figure 8 [5, 31]. On an HS ICEs, the application of a high-reactive blend consisting of methyl ketones not only yielded a higher η_i than conventional diesel but also low engine-out emissions in terms of both NO_x and soot [33]. In addition, the applica-

¹Composition: 50 mol % ethanol, 21 mol % 2-butanone, 15 mol % cyclopentane, 14 mol % cyclopentanone

²Composition: 40 mol % methyl isopropyl ketone, 25 mol % ethanol, 16 mol % methyl acetate, 13 mol % ethyl acetate, 4 mol % pentane, 2 mol % methanol

tion of hydroformylated Fischer-Tropsch (HyFiT) fuels in a vehicle of the current fleet reduced the engine-out particulate matter (PM) emissions by 55–70 % and the CO₂ tailpipe emissions by 3–5 % compared to diesel fuel. Adapting the exhaust gas recirculation (EGR) calibration promised a reduction in NO_x emissions of up to 37.5 % [38]. For the long-term material compatibility of bio-hybrid fuels with engine, fuel cell, and infrastructure components, immersion tests as part of FSC's comprehensive fuel investigations [33, 39, 40] revealed a critical increase in volume of up to 200 %, particularly for molecules with both polar and non-polar functional groups as well as short chain-length molecules that favor diffusion processes into the sealing material [245].

Objectives

Based on the efficiency walk revealed in FSC, the SRA-CFA-2 aims to develop a multi-stage efficiency increase using the concept of fleet compatible fuel and engine co-optimization. In this way, the potential of novel fuels for both the increase of the efficiency and the reduction of pollutant emissions shall be unveiled for engines with and without software and hardware changes. Starting from a simple refueling of the vehicle to unlock the raw fuel influence, the highest efficiency increases and emissions reductions shall be achieved by a dedicated co-optimization of the fuel and the soft- and hardware. This final development stage will be a retrofit solution, adaptable to a wide range of the existing vehicle technologies. For this purpose, the SRA-CFA-2 will (i) identify bio-hybrid fuels and fuel blends that are compatible with the existing vehicle fleet, (ii) co-develop a highly adaptive MCPS design, yielding $\eta_i > 50\%$ for on-road passenger cars, and (iii) enable a [zero-impact emission strategy](#) by combining the MCPS with a tailored and adaptive exhaust gas aftertreatment system.

Work Program

The research will be performed by a close alignment of theoretical investigations, experiments, and numerical simulations within the subtopics combustion concept, exhaust gas aftertreatment, and material & device compatibility.

Based on the MCCS investigations in FSC, the combustion concepts of the MCPSs will be developed, considering the limited degrees of freedom for fleet-compatible engine designs: base engine (peak pressure limit), crankshaft (stroke/bore ratio (s/D ratio)), and cylinder head (gas exchange, charge motion, combustion chamber access). With an increasing degree of effort, (i) the [calibration](#), (ii) the [ignition system](#), (iii) the [injection system](#), and (iv) the [piston](#) remain adjustable. (i): For the calibration settings, the valve timing, the boost pressure, the injection strategy, and the EGR rate will be pre-optimized using numerical simulations (Schröder), fundamental combustion experiments (Pitsch, Kneer), and optical experiments in CVCs and in a single cylinder engine (SCE) (Boxx³, Pischinger). By carefully adjusting the calibration, the heat release in the engine shall be shaped depending on the applied fuel to increase the effi-

³FSC Lighthouse Appointment in 2022: Prof. Isaac Boxx, PhD, Chair of Optical Diagnostics in Energy, Process and Chemical Engineering

ciency of the entire vehicle powertrain. (ii): The MT will be applied as a retrofit ignition source (Pischinger), which has to fit into the spark plug bore. A passive PC is beneficial in terms of packaging and costs. However, we aim to implement an active PC into a series engine to unlock the efficiency potential of the MT revealed in FSC. (iii): For the MT and the MS, injection systems featuring two separate injectors will be developed to fuel the engines with combinations of LR and HR fuels. (iv): The pistons will be replaced to increase the CR. However, the higher CR leads to an increased surface-to-volume ratio and a larger share of crevice volume; thus, impacting the charge motion (Schröder) and increasing the hydrocarbon (HC) emissions as well as heat losses. In order to reduce the HC emissions and heat losses, [combustion chamber coatings](#) will be applied (Pischinger, Heufer, Simon).

The engine-out emissions of the MCPs will be further reduced using exhaust gas aftertreatment measures from FSC. To this end, the fundamental findings on MW-activated exhaust gas catalysis (Simon, [37]) and 3D-printed catalyst carriers (Wessling) will be combined into adaptive retrofit concepts and tested under realistic conditions on laboratory gas test benches (Pischinger), accompanied by multi-scale simulations for a deep understanding of the underlying physico-chemical processes (Khetan⁴).

The vehicle (including the hybrid powertrain operation and the exhaust gas aftertreatment) will be optimized for both the fuel consumption and the pollutant emissions using the vehicle simulation tool chain established in FSC for a virtual calibration (Pischinger). This will also enable the integration of the vehicle into the LCA (see section 4.5.5.3) at an early development stage. Material & device compatibility of new fuel candidates identified in the integrated Fuel & Chemical Design Process (FCDP) will be investigated both numerically and experimentally (Schmitz). For the experimental investigation of the long-term compatibility of novel fuels, new accelerated tests will be developed (Schmitz). The gained comprehensive data base will be utilized for a ML classification based on the molecular character of fuels and sealing materials.

4.5.1.3 Carbon-based Fuel Cells

In FSC², we aim to develop fuel cells with high fuel adaptability. The development of non- or low-noble metal-based catalysts for the anode as well as fuel-resistant cathodes and improved membranes and separators is supposed to improve the overall efficiency. For a broad applicability, we will investigate the whole range of membrane-based low temperature fuel cells, solid-oxide fuel cells as well as microbial fuel cells. The focus in all cases is on [materials with flexible fuel use capabilities](#) as well as designing [fuel-adapted, degradation-optimized operation strategies](#). Also the use of new fuels from the FCDP will be considered to [tailor specific catalyst-fuel interactions](#). The different fuels and their applicability will furthermore be evaluated on the system level to ensure the sustainability of the fuel production, utilization, and possibility for integration into a carbon-hydrogen energy cycle.

⁴FSC Tenure Track Appointment in 2021: Prof. Dr.-Ing. Abhishek Khetan, Junior Professorship of Multi-scale Modeling of Heterogenous Catalysis in Energy Systems

Current State of Research and Previous Work

DLFCs are available in a large variety, utilizing various fuels as well as different reaction conditions, i.e. acidic and alkaline as well as mixed conditions [246]. In preliminary studies, we have identified candidates studied in the literature and characterized them regarding their thermodynamic as well as toxicological data (Figure 10, Mechler⁵). In general, due to the high energy density and easy storability DLFCs are well suited for heavy duty and off-road applications.

A common problem is the poisoning of mostly Pt-based catalysts by intermediates like CO [246]. Non-noble metal catalysts are more poison-resistant and show promising results in alkaline environment [247].

The FSC² clusters vast experience in fuel cell catalyst development and characterization. For instance, we have studied non-noble metal and hybrid catalysts [181, 182] (Mechler, Mayrhofer) as well as noble- and non-noble metal catalysts for both anode and cathode (Palkovits). Also the degradation of electrochemical systems has been studied in-depth with modern technologies such as in-operando mass spectrometry [183] as well as magnetic resonance imaging (MRI) [184], in-operando X-ray computed tomography (XCT) [185], and 3D transmission electron microscopy (TEM) [186].

Besides optimizing the catalyst for given fuel molecules, the latter could also be tailored by fuel design. This has the potential to improve reaction rates by **optimized adsorption on the catalyst surface and simplified bond-breaking reaction-steps**. By now, only few studies have shown that (i) some electrodes can deal with different fuels, hence being adaptive to various resources [248], and (ii) fuel blends can even have advantages over single fuel feeds in terms of performance and cross over [249]. For optimized catalyst-fuel interactions, we can use model-based optimization strategies, where we can build on our capacities in the field of ab initio modelling of heterogeneous electrochemical reactions [187, 188].

Another significant challenge limiting the viability of DLFCs today is the high permeability of fuels through the membranes, which leads to reduced power output [250]. Surface and material modifications, and substitution of perfluorosulfonic acids (PFSA) by hydrocarbon membranes are decisive factors [189]. Improved stability and conductivity as well as a tailored catalyst-membrane interface are needed for successful implementation in real devices. Within FSC² we host a world leading group in membrane formation and characterization, with membrane developments of e.g. PFSA substitutes for acidic as well as alkaline methanol fuel cells [189, 190]. Solid Oxide Fuel Cells (SOFCs) are known for the conversion of carbon containing fuels [251]. Under continuous operation, a lifetime of 100,000h has been shown for a short-stack at the



Figure 10: Illustration of most prominent DLFCs reported in literature.

⁵FSC Tenure Track Appointment in 2020: Prof. Dr. rer. nat. Anna Mechler, Electrochemical Reaction Engineering

FZJ [252], however shut-downs are typically detrimental. Interestingly, the application of reversible operation in Reversible Solid Oxide Cells (rSOCs) has demonstrated the potential to reduce degradation [253]. Thus, investigation on the system level with optimized operation protocols for various fuels or blends that minimize degradation rates is a promising approach. Besides the extensive background of the FZJ in SOFC material development and characterization (cf. also section 4.5.2), we also recently commissioned a test bench for fuel-flexible testing at RWTH. For instance, the add-mix of hydrogen to natural gas has shown significant effects on the operating temperature of the fuel cell, necessitating the development of countermeasures through advanced control strategies.

For sensitive applications microbial fuel cells (MBFCs) can be an attractive alternative, as biocatalysts can operate at ambient conditions without being poisoned by CO and offer the advantage of a membrane-less approach through cathodes and anodes based on highly specific biocatalysts, e.g. lanthanide-containing methanol dehydrogenase (MDH) [254,255]. Also mechanisms observed in MBFCs can be utilized to optimize electrodes for DLFCs. From this, a combination with heterogeneous cathodes in hybrid-fuel cells is possible for improved selectivity and performance. Today, the sophisticated cofactors and structural composition of MDH pose significant challenges to its heterologous production, hampering upscaling and protein engineering efforts. Utilizing our expertise in maturation and folding of multi-cofactor and multi-subunit containing metalloenzymes [191, 192] and collaboration with cooperation partners for MDH-design [255], biotechnological application of MDH in MBFCs can be achieved.

Objectives

In order to develop the next generation DLFCs we strive for a large-picture-approach optimizing the material-fuel system as an interactive core as well as taking into account the system design. Thus, we aim to (i) develop adaptive fuel cells that can work with a variety of fuels and their blends, and (ii) optimize fuel conversion by tailored fuel-catalyst interactions, screening new catalyst materials but also the fuel itself, including the assessment of internally or externally reformed as well as partially reformed fuels. For the material development, the goals are to achieve stable performance with as-low-as-possible noble-metal content, even down to fully non-noble metal approaches, and a special focus to decrease poisoning by intermediate species or cross-over. We will furthermore (iii) optimize membranes for higher stability, reduced fuel cross-over without losses in the high ionic transport performance, and (iv) study and mitigate degradation effects by in-depth structural analysis as well as (v) optimized adaptive operation strategies and showing their feasibility on the system level.

Work Program

Within FSC², we aim to develop fuel cells that are adaptable to a large set of fuels, thus being resilient towards the availability of fuels in the global context. While methanol and NH₃ are currently strongly discussed, we aim to take into account the large variety of possible energy carrier molecules as well as their suitability in terms of energy density, producibility, storability,

and environmental impact (cf. also section 4.5.5). Thus, we are looking for tailored fuel-catalyst interactions, with high conversion rates, decreased poisoning and cross-over, and low environmental impacts.

For advancing the technology, we will investigate catalyst materials both on the anode and cathode as well as developing new membranes based on non-per- and polyfluoroalkyl substances (PFAS) ionomers and with a high fuel tolerability as well as decreased cross-over rates (Mechler, Eichel, Wessling). To identify suitable non-noble metal catalysts, reaction mechanisms will be investigated by identifying adsorbates via in-situ IR- and Raman-spectroscopy (Eichel, Palkovits). Especially similarities for different classes of fuels on model catalysts shall identify unifying mechanisms or intermediates. Identified hurdles in the conversion process of various fuels can be used to predict more suitable material combinations. Using computational predictions of the atomistic surface configurations, optimal host/guest metal combinations will be predicted using the state-of-the-art grand canonical ensemble density functional theory (GCE-DFT) formalism (Khetan). Metropolis Monte Carlo simulations based on the cluster-expansion method calculations (CEMC) will be employed to determine the ideal alloying ratios that result in optimal equilibrium surface configurations. These can then be prepared by the flexible catalyst synthesis platform as utilized in section 4.5.3 (Palkovits). On the cathode side, catalysts that are resistant to any remaining fuel cross over are essential. Single-metal catalysts in a carbon matrix are promising candidates, as they are insensitive to most C-containing impurities. Their stability will be further improved by combining them with co-catalysts in a hybrid approach (Mechler). Material characterization will span from lab scale characterization, over single cells up to the device level. Here, also the impact of reaction conditions, especially fuel concentrations and combinations will be studied. Degradation effects will be studied from the catalyst up to the cell level, utilizing in-operando spectrometry & tomography (Eichel). To ensure long-term operation of all components of a fuel cell system, the stability of sealings, tubes, and membranes will be investigated experimentally as well as by theoretical predictions (Schmitz).

Ion-exchange membranes not only need to be stable under operation with various fuels, but are also required to decrease the cross over of fuels, products, and reaction gases. We will hence investigate the modification of existing membranes as well as the development of new PFAS-free ionomers and membranes (Wessling, Eichel). While cation-exchange membranes are conventionally utilized in alcohol fuel cells, anion exchange membranes (AEMs) as well as bipolar membranes (BPMs) open the space for a larger variety of catalysts and operation modes. Besides experimental investigations of mass-transfer and degradation mechanisms, MD simulations will be utilized to determine sources of fuel permeation and electro-osmotic drag (Wessling). This will be assisted by Chemical-Color-Coded Non-equilibrium molecular dynamics (CCC-NEMD) simulations under applied electric fields of varying strengths to elucidate the mechanisms of ion transport through various candidate membrane materials (Khetan). The effects of membrane structure, charge density, and functional groups on ion selectivity and permeability will be performed using trajectory analysis.

For a power- and fuel-flexible operation of SOFCs, we aim to develop dynamically-customizable

protocols that minimize degradation on a system level. We will utilize the process of reversible operation to refine reversible cycling protocols to establish optimal conditions that enhance performance while minimizing degradation. To this end, we will design and employ accelerated stress tests (ASTs) along with advanced characterization techniques such as X-ray diffraction (XRD), transmission electron microscopy (TEM), and electrochemical impedance spectroscopy (EIS) to monitor changes in material structure and electrochemical behavior. Computational modeling will support these efforts by simulating degradation pathways and enabling predictions that mitigate operational stresses on cell integrity. Furthermore, we aim to find customization criteria based on various fuels and fuel blends. Complementary online gas composition analytics, including Fourier-transform infrared spectroscopy (FTIR) and non-dispersive infrared (NDIR), will be utilized to develop tailored after-gas treatment strategies. Adaptive strategies within the parameter space of efficiency, emission and reversible operation will establish a low-degradation mode irrespective of the fuel. This enables the assessment of integrating the fuel flexible rSOCs into existing energy infrastructures including the heavy-duty transportation (Pischinger).

For remote applications and limited purities, MBFCs will be investigated (Lauterbach). The co-synthesis of maturases and chaperones should enable the heterologous production of MDH for upscaling, protein engineering and use in membrane-less MBFCs. Either a mediator such as osmium or conductive polymers such as polypyrrole or polyaniline will be used for the anode [256]. In addition, electron transfer to the anode will be improved by amino acid exchanges on the surface for orientated immobilisation, lowering the distance between cofactor and electrode according to Marcus theory, and developing a fusion protein from MDH and the cytochrome c domain.

By investigating the whole breadth of DLFCs we aim to identify the best option for each application. With a tailored fuel-catalyst optimization in all fields, best-case scenarios can be determined, while a fuel-flexible, adaptive operation is still ensured. [To strengthen this new research area within the FSC², a new lighthouse professorship in the field of Electro-Organic Molecular Transformations will be established.](#)

4.5.1.4 Proposed Staff and Funding of SRA-CFA

Table 4.5.1.1: Proposed Staff in SRA-CFA⁶

Staff category	2026	2027	2028	2029	2030	2031	2032
	Number of persons						
Postdoctoral researchers	2	2	2	2	2	2	2
Doctoral researchers	10	10	10	10	10	10	10

⁶Proposed staff funded by DFG solely comprises costs for scientific personnel for the planned research activities. For additional staff engaged in FSC² but funded by the participating institutions see Section 6.2.

Table 4.5.1.2: Funding Request for SRA-CFA⁷

Funding category	2026	2027	2028	2029	2030	2031	2032
	Totals per year in thousand euros						
Staff (Total for 4.5.1)	859	876	894	912	930	949	968
Direct project costs (excluding staff)	363	278	238	138	138	138	138
Total instrumentation < €150,000	100	197	50	0	55	0	0
Total instrumentation > €150,000	170	160	0	0	0	0	0
Femtosecond optical parametric amplifier	170						
Fuel cell test station		160					

Instrumentation below 150 000 €

A high-speed image intensifier (117 k€) will be used to visualize low-luminosity flames, e.g. very lean flames or hydrogen flames. To investigate the combustion chemistry with respect to single species, these species can be directly measured in RCMs and in STs by using laser absorption spectroscopy. Currently, the IR-laser system is used with a central wavenumber of 1740 cm^{-1} , enabling the measurement of carbonyl-bond stretching. To measure typical engine-out emissions, such as ethylene and N_2O , the procurement of a new system with a central wavenumber of 1200 cm^{-1} is required (50 k€). To investigate the combustion chemistry using multisampling of combustion gas, the procurement of a gas measurement system is intended (55 k€), in which the samples are stored in sample loops and then automatically introduced into the measurement system of the gas chromatography and mass spectrometry. For the investigation of wall coating effect on the surrounding gas, a microscopic fiber-based cavity-enhanced spectroscopy system is required (100 k€). To investigate novel liquid fuels on newly developed ion exchange membranes for fuel cells, the experimental periphery for the measurements has to be extended (80 k€).

Instrumentation above 150 000 €

To investigate the evaporation, mixing, ignition, and combustion dynamics of hydrocarbon fuel injected into ammonia and ammonia-hydrogen fueled ICEs, detailed laser-, optical-, and spectroscopic measurement techniques will be applied to characterize local temperature, composition, reaction rates, and heat-release rates. To obtain quantitative, 2-dimensional measurements of the combustion radicals H, O, and N, which are known to drive the coupling of hydrocarbon and ammonia chemistry, a femtosecond optical parametric amplifier (170 k€) will be procured. For the evaluation of new fuel cell materials and fuels for electrochemical energy conversion an automated fuel cell test station is needed which can operate with various organic fuels. This includes all the necessary periphery, a high-current potentiostat with EIS capacities and an central automation platform for save long-term operation (160 k€).

⁷For costs of personnel, an annual increase of 2% is assumed based on the DFG rates for 2024. Direct project costs include travelling, standard small equipment and consumables.

4.5.2 SRA "Ammonia Fuel Utilization" (SRA-AFU)

PIs: [Pitsch](#), von der Aßen, Eichel, Mechler, Palkovits, Pischinger, Simon; ARs: Boxx, Khetan, Kneer, Schmitz, Schröder

The SRA-AFU develops clean and efficient systems for thermochemical and electrochemical conversion of ammonia (NH_3). Compared with hydrogen, ammonia has the advantage that it can be liquefied at moderate pressures, which makes it well-suited for easy and inexpensive long-distance transport and long-term storage [257]. Also, its production is well understood and can be carbon neutral if based on renewable energy. For utilization, NH_3 can be reformed to H_2 for use in ICEs or after purification in proton exchange membrane fuel cells (PEMFCs). However, while the toxicity of NH_3 limits its use to well-controlled environments, direct thermochemical and electrochemical energy conversion in ICEs and high- and low-temperature fuel cells is of interest for marine and stationary applications due to the higher overall efficiency potential [258]. Yet, NH_3 has unique thermodynamic, physical, chemical, and electrocatalytic properties differing significantly from those of conventional fuels causing significant NH_3 -specific challenges, which will be addressed in SRA-AFU considering ICE, fuel cells, and exhaust-gas aftertreatment for both applications. For the thermochemical conversion of NH_3 in ICE, the low reactivity and high fuel-nitrogen content can lead to unstable combustion, low efficiency, NH_3 slip, and emissions of NO_x and N_2O . These issues will be tackled by exploring different combustion modes, tailored injection and mixing concepts, and adjustable reactivity enhancement, covering fundamental aspects all the way to the improvement of NH_3 engine efficiency with near-to-zero engine-out emissions. The electrochemical conversion of NH_3 in fuel cells exhibits risks of NO_x formation in high-temperature fuel cells and catalyst poisoning and membrane degradation in low-temperature fuel cells. Non-noble metal catalysts, tailored membranes with lower cross-over, proton-conducting ceramic membranes, as well as poisoning and degradation mechanisms will be investigated to resolve these issues. For the critical aftertreatment of the complex exhaust gas mixtures from both ICEs and fuel cells, new catalyst materials for NH_3 -slip treatment and coupled N_2O decomposition and NO_x reduction in both conventional and microwave-stimulated systems will be developed using a combination of experimental and numerical methods.

Strategy and Structure of the SRA-AFU

The structure of this SRA is shown in Figure 11. We consider thermochemical and electrochemical energy conversion of NH_3 as well as emission control, which is relevant for both. The sub-SRA "ammonia combustion" will address the critical aspects to enable highly efficient and clean NH_3 engines through comprehensive experimental and numerical investigations.

Different engine technologies will be pursued based on the MT concept in combination with reactivity tailoring by partial onboard or in-engine NH_3 reforming, and based on high compression ratio MS engines with in-cylinder fuel staging. Novel injection methods for NH_3/H_2 -blend injection will enable tailored mixing and staging strategies. The SRA-AFU will exploit all degrees of freedom to develop both retrofit and novel NH_3 -engine concepts.

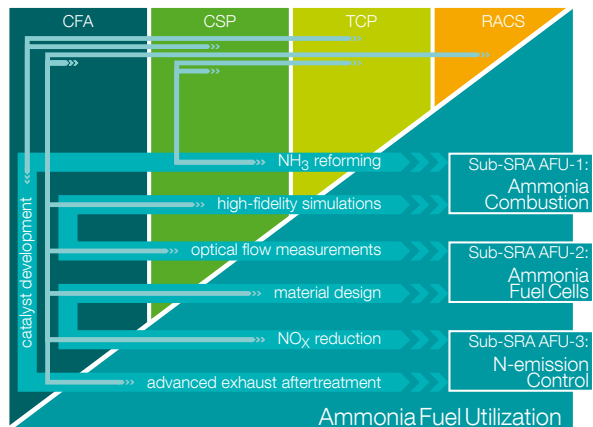


Figure 11: Structure of the SRA-AFU

igated by adaptive operation and exhaust gas aftertreatment or by direct prevention using solid proton-conducting fuel cell (SPCFC). Both direct SOFC and SPCFC concepts will be considered here. The sub-SRA “N-emission control” addresses the exhaust gas aftertreatment for NH_3 engines and SOFC fuel cells. Advanced durable catalysts will be developed capable of handling wide variations in exhaust composition with a focus on N_2O and ammonia reduction, which will be enabled using novel microwave-assisted technologies. The challenges of enhancing efficiency and reducing emissions in thermochemical and electrochemical NH_3 conversion will be addressed through strong interactions within FSC². Additional connections exist with SRA-CFA in the investigation of flame-wall interactions, emission control, and material compatibility, with SRA-CSP on ammonia activation, and with SRA-RACS to integrate considerations of efficiency, resilience, adaptability, and environmental sustainability into the development of NH_3 fuel utilization technologies.

4.5.2.1 Ammonia Combustion

This sub-SRA focuses on two major tasks: Improving the operational stability and efficiency of NH_3 engines and reducing engine-out emissions. In the FSC, we successfully developed lean-burn bio-hybrid fuel concepts using MT ignition strategies combined with catalytic and thermal coatings to enhance ignition and combustion of low-reactivity lean mixtures. These concepts provide a powerful toolset as a starting point for facilitating NH_3 -based combustion. In addition, tailored onboard reforming of NH_3 will be used to generate H_2 as a highly reactive fuel component. Novel injection and mixing strategies, and intrinsic-instability controlled combustion concepts will be exploited to enhance reactivity and support NH_3 -specific targeted advanced combustion concepts. To fully exploit the potential for developing novel NH_3 engine concepts and technologies, we will conduct fundamental experimental and numerical investigations into catalytic NH_3 reforming, injection of NH_3/H_2 blends, catalytically and temperature-controlled pre-chamber combustion, and intrinsic instability-enhanced combustion for NH_3/H_2 blends. Further, high-fidelity simulations with physics-based and data-driven modeling will complement device and system-level experiments for optimizing device design and operation, considering unstable combustion, efficiency, emissions, and sustainability.

The sub-SRA “Ammonia Fuel Cells” focuses on increasing NH_3 fuel cell efficiency and durability. Both low- and high-temperature fuel cells will be considered. For low temperature direct ammonia fuel cell (DAFC), efficiency is a challenge. We will exploit the great potential with new poison-resistant catalyst materials for ammonia oxidation reaction (AOR) and oxygen reduction reaction (ORR), as well as with improved AEMs. For direct NH_3 SOFC, a challenge is the potential formation of nitrogen oxides. This can be mit-

Current State of Research and Previous Work

Bio-hybrid fuels and their performance in ICEs have been systematically explored in the FSC. Methanol was shown to be an excellent choice as an alternative fuel when used in a tailored engine with indicated efficiencies of close to 50 % for a passenger car engine and even higher than 50 % for heavy-duty engines. The advantages of methanol are related to a combination of outstanding knock resistance with high burning velocities [41]. Interestingly, NH_3 has an even higher octane number and ignition temperature, making it highly knock-resistant. However, the chemical properties of NH_3 pose severe challenges for applications in engines: (1) Because of its low reactivity, NH_3 is difficult to ignite, which can cause unstable combustion; (2) NH_3 has very low laminar flame speed, impacting stability and efficiency, and (3) the fuel-inherent nitrogen promotes the formation of nitrogen oxides and the large quenching distance can cause NH_3 slip. [The proposed work will address these challenges through fundamental investigations and new technological concepts, fostering highly efficient and stable combustion with near-zero emissions.](#)

Dual-fuel concepts have been proposed to compensate for NH_3 's slow flame propagation by introducing hydrocarbon fuels or H_2 [259]. The latter is particularly interesting since the process remains carbon-free, and H_2 can be produced onboard via the reforming of NH_3 with a catalyst driven by exhaust gas heat. A 10 % rate of NH_3 reforming, for instance, was found to enhance the engine's range of stable operating conditions significantly [259]. On the other hand, H_2 -rich blends tend to increase NO_x and N_2O emissions [259]. The proposed work will consider onboard and engine-internal partial catalytic reforming of NH_3 . Catalytic NH_3 reforming has already been investigated in previous work [42] [193], where a Fe_3N nano-particle sponge was shown to be a promising catalyst. Staged combustion of NH_3 has shown advantages in reducing NO_x emissions and NH_3 slip in stationary gas turbines [257]. Thus, staged combustion concepts in ICEs are considered to have great potential to reduce engine-out emissions. However, the NH_3 injection process, which is of crucial importance for such a combustion strategy, is poorly understood due to NH_3 's unique physical properties [260]. Thus, the proposed work will investigate various engine combustion concepts and injection strategies for NH_3 and NH_3/H_2 blends. In addition, simulation-based design is an essential tool for device and process design, but modeling $\text{NH}_3/\text{H}_2/\text{N}_2$ -air flames poses significant challenges due to the unique intrinsic instability-induced highly non-linear turbulence-flame interactions, as well as the complex flame-wall interactions and formation of nitrogen-containing pollutants.

In our previous work, the complex combustion behavior of NH_3 and NH_3/H_2 blends has been investigated from a chemical kinetics point of view, for instance, by measuring laminar burning velocities of NH_3 /air flames under microgravity conditions in drop tower experiments [43] and developing comprehensively validated chemical kinetic models [23,44]. In other work, premixed NH_3/H_2 flames were observed to develop intrinsic flame instabilities, resulting in significantly increased fuel consumption rates, overshoots in local flame temperature and NO_x formation, and local extinction, as seen in the direct numerical simulation (DNS) results shown in Figure 12.

4 Research Program

In addition, the research facilities already established in the FSC provide a powerful toolset for investigating NH_3 -based combustion. These include the thermodynamic and optical engines for performance, efficiency, and emission characteristics [6, 7, 29], a multifunctional high-pressure burner facility (MHBF) and a turbulent compression reactor (TCR) for turbulent reactive flow characterization, a femtosecond two-photon laser-induced fluorescence (LIF) method for temporally-resolved measurements of flame structure and dynamics [45, 46], catalytic in-cylinder coatings for reducing flame quenching distance and incomplete combustion [47], a transparent nozzle setup for measurements of nozzle-internal flow phenomena [48], and adaptive-mesh simulation tools for highly accurate numerical investigations of fuel sprays, flash boiling, and engine combustion [49, 50].

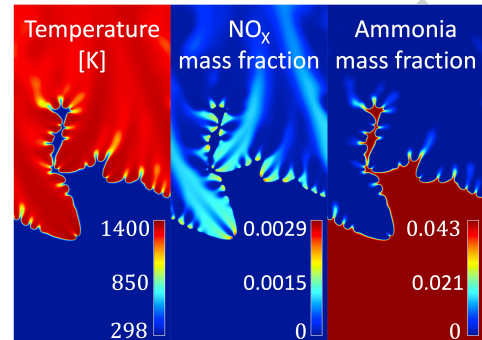


Figure 12: DNS of laminar $\text{NH}_3/\text{H}_2/\text{air}$ flame with 40 mol-% H_2 showing intrinsic flame instabilities without which the flame would appear as a horizontal line.

Objectives

The aim of the sub-SRA “Ammonia Combustion” is to enable heavy-duty NH_3 engines with stable combustion, high thermal efficiencies, and near-zero emissions. The main objective is to develop integrated NH_3 -specific engine concepts including (i) partial on-board and in-engine NH_3 -reforming using highly active and selective catalysts to provide on-demand $\text{NH}_3/\text{H}_2/\text{N}_2$ mixtures, (ii) advanced MT concepts using catalytic surfaces and controlled pre-chamber heating, (iii) knowledge-based triggering of intrinsic flame instabilities to increase combustion speed, and (iv) new NH_3 and NH_3/H_2 -blend injection concepts in MS engines enabling in-cylinder combustion staging with tailored stratification to suppress fuel slip and nitrogen oxides formation, and increase efficiency. This will be supported by advanced quantitative characterization methods and modeling of the interactions of the individual processes, including reforming, injection, mixing, and combustion. Based on the resulting knowledge and numerical models, computational design and system-level experiments will be performed to achieve the global optimization of the entire combustion system.

Work Program

The potential for enhancing efficiency and mitigating engine-out emissions will be explored with a hierarchy of methods and technologies. Different engine concepts and fuel injection strategies will be considered as shown in Figure 13. MT engines will utilize on-demand reformed H_2 or high-reactivity bio-hybrid fuels as ignition accelerators, pre-chambers with catalytic surfaces and active heating potentially enabling auto- instead of spark-ignition thereby reducing pre-chamber volume and efficiency losses. MS engine concepts will rely on targeted in-cylinder staging with novel high-pressure injection strategies for NH_3/H_2 blends.

Catalytic on-board NH_3 reforming, either prior to intake or in-engine will be studied (Palkovits) as

a central element of the proposed combustion concepts. A data-driven approach will support the multivariate design of tailored high-entropy alloys and single-atom catalysts through combined high-throughput screening and ML-accelerated computational studies. The derived structure-activity relations also provide insights into catalytic structures for NO_x and NH_3 -slip abatement. Advanced pre-chamber and cylinder catalytic coating materials will be synthesized in-house (Simon) building on our experience [47]. Here, we will primarily focus on oxide and the relatively unexplored nitride catalysts to engage their surface available O- and N-atom vacancies as active sites.

For the (partially) premixed combustion concepts in the MT engines, it is crucial to quantitatively characterize the combustion behavior of fuel blends with varying H_2 content, especially for the effective utilization of the intrinsic instability-controlled flame propagation. This will be accomplished by fundamental investigations with various experimental facilities (Boxx, Pitsch) and spatially and temporally highly resolved DNS based on a hierarchical approach (Pitsch). An MHBFB will be employed for fundamental studies on the effects of turbulence, flame intrinsic instabilities, pollutant formation, and their interactions in turbulent jet flames. Various pre-chamber-based MT combustion configurations, including premixed and partially premixed flames using combinations of low-reactivity (NH_3) and high-reactivity (H_2 , bio-hybrids) fuels will be investigated.

In particular, incomplete combustion of NH_3 -rich mixtures in the pre-chamber will generate hot jets with high H_2 concentration, leading to enhanced combustion in the main chamber. Both DNS as well as laser-diagnostic experiments in the TCR will be performed focusing on the intricate interplay of mixing, auto-ignition, and flame propagation with turbulence and flame stretching. Temperature and species distributions will be quantitatively localized by single-shot 1D Raman spectroscopy and femtosecond two-photon LIF, providing the number density of important species, such as NH_3 , NH , and atomic N, O, and H, during molecularly controlled ignition and turbulent flame propagation of NH_3/H_2 blends (Boxx). Such advanced high-resolution diagnostics will also be applied to device-level experiments, including optical engines. DNS will also be used to reveal the flame speed boosting effects by differential diffusion-induced intrinsic instability, and the effects of catalytic wall coating on near-wall mixture composition, flame dynamics, and flame-wall interactions, which will be investigated jointly with the SRA-CFA. The DNS will support the development of high-fidelity large eddy simulation (LES) models for computational design and optimization at both device and system levels (Pitsch).

The MS combustion concept with various fuel injection strategies enables diffusion and staged

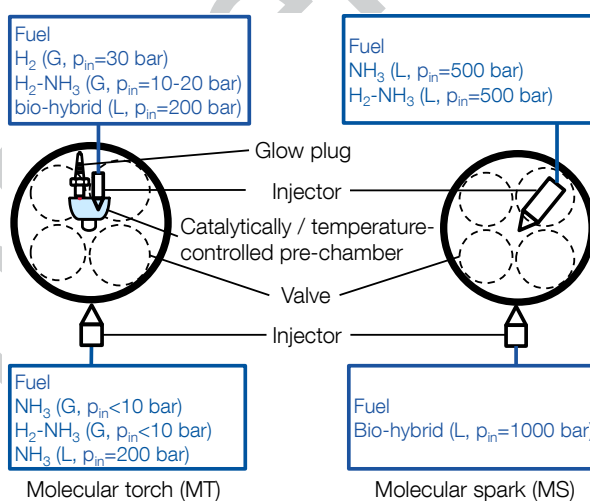


Figure 13: Ammonia engine concepts. 'L' stands for liquid, 'G' for gaseous, and ' p_{in} ' for injection pressure.

combustion through targeted fuel placement and mixing strategies, potentially avoiding flame wall quenching and achieving high efficiency with low NH_3 slip. Pioneering injection and mixing concepts will be employed to facilitate tailored mixture preparation of NH_3/H_2 blends for various applications and operating conditions, either through nozzle-internal mixing or by dissolving gaseous H_2 into liquid NH_3 . Particular emphasis will be placed on the injection of single or two-phase NH_3/H_2 mixtures at high pressures of up to 500 bar for both concepts, allowing for proper mixing of the fuel blends and fast diffusion combustion at high compression ratios. The associated highly transient thermophysical and fluid dynamic processes, such as dissolution limits, degassing, decompression, and flash-boiling will be described and quantified based on a hierarchical ensemble of experimental (Kneer) and numerical (Schröder) investigations, covering studies on single droplets, droplet streams, nozzle-internal mixing and degassing, as well as jets and sprays in high-pressure chambers.

Based on the fundamental quantitative characterization of the individual processes, promising reforming, mixing, and combustion strategies will be proposed and tested in full-system thermodynamic and optical engine layouts (Pischinger). Well-designed engine operation conditions will be investigated considering the non-linear coupling of the underlying processes, such as the temperature and pressure dependence of intrinsic instabilities and flash boiling, turbulence interactions with the MT and MS, and the effects of mixing and flame dynamics on pollutants. Computational design using high-fidelity LES and optimization approaches will be closely integrated into the experimental investigations to understand in-engine processes and efficiently achieve a global optimization of the combustion system (Schröder). The injection of single or two-phase NH_3/H_2 mixtures and the combustion with intrinsic instabilities exceed the capabilities of current numerical models. Therefore, novel LES models, based on fundamental experimental and DNS investigations, will be developed and employed. Artificial intelligence (AI) hold great promise for modeling multi-physics flows, in particular in the cases where the complexity of the physics impedes traditional physics-based modeling from first principles. A junior research group (JRG) "AI in reactive fluid dynamics" will be established, focusing on the data-driven modeling for multi-physics reactive flows in ammonia engines and fuel cells.

4.5.2.2 Ammonia Fuel Cells

As an alternative to combustion, the chemical energy stored in NH_3 can be directly harvested in DAFCs. In low-temperature DAFCs, NH_3 is converted catalytically. In SOFCs operating at high temperatures, NH_3 reforms internally to N_2 and H_2 , which is then converted in the fuel cell process. DAFCs have the potential for higher overall efficiencies, as the intermediate step of external NH_3 reformation is omitted and, in case of SOFCs, the heat from the exothermic fuel cell reaction can be directly utilized by the endothermic ammonia decomposition. Within FSC², we will investigate both low- and high-temperature fuel cells with [highly active and selective catalysts that are resistant towards poisoning by \$\text{NH}_3\$ or reaction intermediates](#). Furthermore, [tailored separators and membranes, as well as adapted operation strategies](#) will be developed to mitigate degradation and side-product formation. The aim is to improve performances and

economic viability as well as to reduce cross-over, poisoning, and to avoid or mitigate NO_x formation.

Current State of Research and Previous Work

The concept of DAFCs has already been proposed about 50 years ago for both low-temperature [261] and high temperature applications [262]. Nowadays, the already utilized Ni-based electrodes show high NH_3 decomposition activity [263]. However, in conventional SOFCs, utilizing oxide-conducting ceramics like yttrium-stabilized zirconia (YSZ), NH_3 can directly react with the O^{2-} to form NO_x [262]. Here, aftertreatment is necessary to remove NO_x as well as unprocessed NH_3 . Alternatively, SPCFCs can be utilized, where H^+ is transported from the anode to the cathode, thus avoiding NO_x formation. While SPCFCs benefit from lower operation temperatures [264], this also causes new challenges, for instance, the need for improved catalyst activity [265]. Typical materials for SPCFC electrolytes are yttrium-doped barium zirconate (BZY), yttrium-doped barium cerate (BCY) and yttrium-doped barium zirconate-cerate (BCZY) [266]. Within the cluster, we combine extensive experience in the field of material and cell development for SOFCs [195] with competences in the operation of fuel cell test benches [196] as well as fuel cell simulation addressing system performance, locally resolved electrochemical cell behavior, and mechanical stress distribution within the different cell materials [197–199]. First SPCFC separators have been developed with promising results at 600 °C [194] (Figure 14), and under NH_3 -operation [200].

For low-temperature fuel cells, recent works have shown promising results achieving power densities exceeding 100 mW/cm^2 (up to 420 mW/cm^2) from a single cell. However, these studies typically utilize platinum-based catalysts [267]. Another critical factor of noble-metal catalysts is the risk of catalyst poisoning. Thus, non-noble metal alternatives, especially based on Ni in alkaline environment, have been explored [268]. Most Ni-based materials currently face the issue of high AOR onset potentials, which not only reduces efficiency but also imposes a risk for the formation of NO_x [269]. We believe that an unexplored potential is the use of single-atom metal catalysts in carbon- as well as metal-matrices and their further combination to hybrid catalyst materials. Such an approach has been successfully applied previously in H_2 fuel cells [201]. In preliminary studies, Ni- and Ni-Cu-hydroxides were investigated as catalysts for AOR. It was found that the Ni-Cu hydroxides possess better catalytic activity than pure NiOH_2 for AOR. Additionally, supporting them on reduced graphene oxide (rGO) and carbon nanotubes (CNT) as conductive supports further increased their performance (Figure 15).

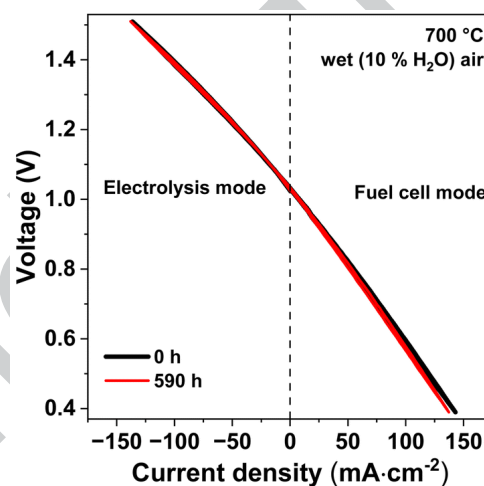


Figure 14: *iV* curves before and after 590 h in electrolysis operation of an electrolyte supported PNO/DNSYYb/Ni-BZY cell, showing the possibility of stable operation of SPCFCs [194].

4 Research Program

Furthermore, the search for AEMs that are long-term stable in the NH_3 environment is still a challenge. Within FSC² we can build on long-term experience in membrane engineering of proton- as well as anion conducting ionomers, where a significant decrease of cross-over in DLFCs was proven (cf. section 4.5.1). The use of a potentially liquid fuel in comparison to gaseous hydrogen furthermore requires the rethinking of the fuel cell design, for instance, in terms of electrode geometry, electrolyte distribution, and water management. Here we can harvest our experience in the computational and experimental evaluation of various flows, including both single phase as well as mixed liquid-gas-phases in electrochemical environments [51] (Schröder).

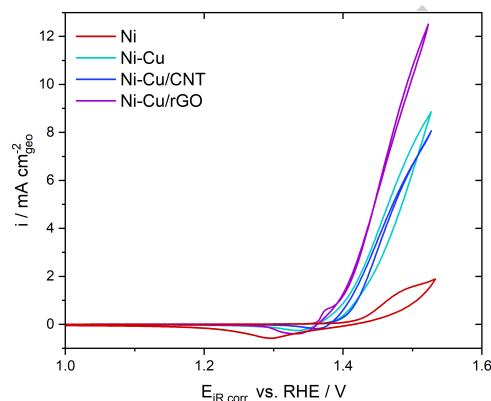


Figure 15: Rotating disc electrode measurements in 1 M KOH + 0.5 M NH_4OH for Ni- and Ni-Cu-hydroxides and the impact of supporting them on CNTs and rGO.

Objectives

DAFCs are identified as a potentially highly efficient technology for direct NH_3 valorization. Next-generation systems will be developed by innovative material and operation concepts, which in a combined effort shall improve efficiency with low cross-over and degradation rates. Single- and biatom metal catalysts as well as hybridization strategies contribute to reduced overpotentials and minimize poisoning. PFAS-free AEMs will be developed to reduce the cross-over of ammonia and for improved live-time under the demanding NH_3 operation. NO_x formation in high-temperature fuel cells will be tackled by adaptive fuel compositions and blends, off-gas characterization and treatment, as well as development of new components, specifically SPCFCs with metal-ion-doped, ceria-based proton-conductors. Overall, we aim to develop **NH_3 -ready fuel cell systems with minimized cross-over and NO_x formation, and with efficiencies surpassing the combination of NH_3 -reformation with conventional PEMFCs.**

Work Program

Both SOFCs and SPCFCs are promising technology solutions for NH_3 -conversion. For SPCFCs, we will go beyond conventional Ni-gadolinium-doped ceria (GDC) based electrodes by utilizing samarium- and praseodymium-doping, as they promise higher ionic and electronic conductivity. Further, doping with Fe will be investigated to enable NH_3 decomposition at the lower operating temperatures of SPCFCs. Besides developing improved electrode materials, the resistance of the proton-conducting separators themselves needs to be enhanced, e. g. by reducing the electrolyte thickness. To stabilize thinner electrolyte layers, we will develop fuel electrode supported SPCFC cells, which requires sophisticated coating methods such as tape-casting for the production of technically relevant scales. To optimize thermal and chemical expansions, sintering activity, and mechanical properties of the materials, we will tune material combinations as well as sintering and tape-casting conditions. Electronic leakage will be addressed by introducing a

GDC barrier layer between electrode and electrolyte. We will also investigate the extent of nitridation by the direct NH_3 -utilization and its effects on performance and long-term stability. The performance and stability of the new materials and cell manufacturing in DAFC is investigated in-operando by current-voltage characteristics and EIS. Combined with advanced ex-situ and in-situ analysis (e. g., focused ion beam - scanning electron microscopy (FIB-SEM) tomography and high-temperature TEM), the degradation can be assessed and mitigated (Eichel). The use of partially reformed NH_3 in SOFCs is another strategy to improve performance and reduce NO_x formation. Furthermore, H_2 can also be generated when utilizing the system in electrolysis mode. We will utilize such a reverse operation for a load-flexible operation and further integrate this into optimized operation strategies to reduce long-term degradation rates. For an online monitoring of gas compositions under varying operating conditions, we will develop advanced online monitoring technologies, including FTIR and NDIR sensors (Pischinger). We will investigate various operating conditions by assessing and comparing the performance of cells fueled by partially or fully pre-reformed NH_3 versus complete internal reformation, as well as fuel blends, particularly hydrogen-ammonia fuel blends. This part will focus on understanding how ammonia and hydrogen interact within the cell environment and influence performance metrics such as efficiency, stability and endurance. For low-temperature fuel cells, [material development](#) will focus on catalyst and membrane design. For the latter, we will introduce PFAS-free ionomers with decreased cross-over towards both carbon-based fuel as well as NH_3 conversion intermediates (cf. SRA-CFA, Wessling). For catalyzing the AOR, we have shown that non-noble metals can be promising alternatives to noble-metal catalysts, such as Pt and Ir, typically used on for anode and cathode of DAFCs. We will further tune the activity by variations in the material composition, crystallinity, and utilization of conductive supports. [Single- and biatomic catalysts](#) are promising next-generation catalysts, as they can provide active metal centers in elevated oxidation states necessary for AOR at low onset potentials (Mechler). The electronic environment can be modified by the addition of the doping-ions P, S, and B. To strengthen this necessary core expertise, [a JRG will be established with a special focus on catalyst development and testing for low-temperature DAFCs](#). Further promising catalyst materials can be expected from insights developed in the SRA-CSP on the activation of NH_3 (Palkovits) based on their synthesis platforms as well as theoretical predictions of novel catalysts from density functional theory (DFT) calculations on those single-atom catalysts (Khetan). Non-noble metal catalysts will furthermore be utilized as ORR-catalysts for the cathode, as they provide advanced poison-resistance over conventional Pt-based materials. Utilizing hybridization concepts of single- or biatomic catalysts on both the anode as well the cathode side with small amounts of noble metals can further boost their performance and long-term stability. This will allow to produce non- or low-noble metal DAFCs, overall lowering the costs of these systems without compromising on their performance. Their feasibility will be tested by manufacturing full electrodes. For those, the higher catalyst loadings require dedicated electrode designs, tuning the mass-transport in the porous structure by optimized ink formulations and electrode manufacturing methods (Mechler, Wessling). The fuel cell will further be optimized for improved mass-transport of reactants and products with [tailored flow-fields and electrode structures](#). This is supported by numeri-

cal simulations and micro-particle image velocimetry (PIV) experiments for volumetric flow field measurements in narrow channels and channel structures, as well as experimental analysis of the interaction of gas bubbles and fluid flow (Schröder). Fundamental findings will be transferred to single-cell testing. Here, insights on the impact of [realistic operation parameters](#) on the performance and stability of catalyst materials will be gained. Conducting design-of-experiment studie with the support of SRA-RACS will open the possibility to optimize reaction conditions within short time-frames.

4.5.2.3 N-emission Control

While commercially available exhaust after-treatment systems (EATSs) can deal well with NO_x , reducing the unusually large NH_3 -slip from incomplete NH_3 combustion and N_2O as a highly potent greenhouse gas are still unresolved challenges. To address the issue of NH_3 -slip, we will use highly specific absorption materials, which can allow for an efficient separation of the slipped NH_3 from the other exhaust gas constituents. We will also explore the use of catalytic reformers for decomposing the slipped NH_3 into N_2 and H_2 . To address the most difficult challenge of N_2O decomposition, we will develop new catalyst materials with no or low-precious metal content that can perform coupled $\text{NO}_x+\text{N}_2\text{O}$ removal at technologically relevant conditions. We will also explore unconventional methods like MW activation, which have shown promise in aiding heterogeneous catalytic reactions but have yet to be employed for N_2O treatment. Finally, we will develop new setups for spectroscopic operando monitoring of reaction intermediates and perform accelerated reactive MD simulations, which will lead to a deeper “in-operando” understanding of the catalytic interfaces and the reaction mechanisms.

Current State of Research and Previous work

The FSC has developed innovative EATSs to reduce emissions such as CO, NO_x , and unburned hydrocarbons, for the combustion of bio-hybrid fuels in ICEs [47, 52, 53]. We have made key contributions to the fundamental understanding of Cu-based zeolites as effective catalysts for NO_x reduction at 200 °C and below [54, 55]. Our investigations have elucidated the intricate dependence of the catalytic activity on the Cu-ion mobility, which was itself found to be non-linearly dependent on temperature [54, 55]. However, these catalysts are mostly inactive for N_2O decomposition at such low temperatures. Our previous work [52, 53] indicates that the efficient decomposition of N_2O is facilitated only above 450 °C.

The best known N_2O decomposition catalysts are comprised mainly of precious metals. Thus, new low-temperature catalysts need to be developed with no or low precious metal content that allow for coupled De NO_x -selective catalytic reduction (SCR) and N_2O decomposition under technologically relevant conditions [270]. These conditions also include the inhibitory effects of O_2 , NO_x , and H_2O , which are poorly understood [271]. It is also essential to deal with the large NH_3 -slip as transient combustion in an ICE exhibits disparate NH_3/NO ratios with reported values even larger than unity [272]. Conventionally, NH_3 -slip catalysts utilized in automotive applications also form secondary NO and N_2O , thus posing further problems downstream. There-

fore, either storing NH_3 or further reforming NH_3 into N_2 and H_2 with high selectivity are both sensible and necessary.

Recently, we employed the ab initio energetic span model (ESM) to analyze N_2O decomposition activity on pure and hybrid catalysts [56]. Our work revealed excellent opportunities for enhancing N_2O decomposition by exploiting weak correlations between adsorption free energies of intermediates. It also offered a thermodynamics-based explanation for the inhibitory effects of NO on N_2O decomposition. Nevertheless, the operando surface of the catalyst has many interacting intermediates, whose reaction kinetics are strongly dependent on the coverage. A fundamental investigation of these effects can help design catalysts that work under technologically relevant conditions.

As a significant step forward for shortening the cold-start phase in EATSs, we recently introduced a MW-assisted catalytic setup [37], as shown in Figure 16. Using CO oxidation as a model reaction, this effort not

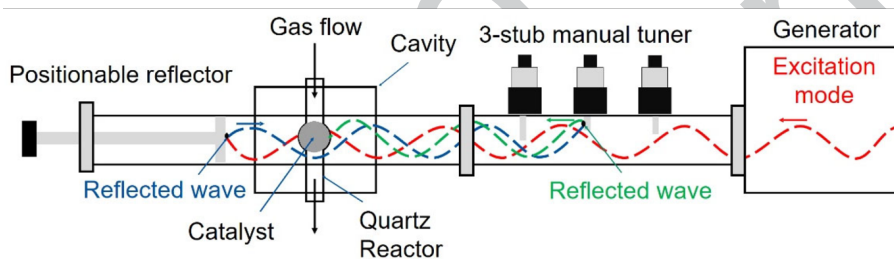


Figure 16: Schematic representation of the monomode MW-catalysis setup from our work [37] in which the MW-power directed towards the sample is maximized, while the power reflected back to the generator is minimized.

only achieved enhanced conversion rates but also highlighted the critical importance of the catalyst temperature distribution, thermal runaway, hotspot formation, particle size effects, gas flow and system design, all of which will be useful for the development of the target EATSs.

Objectives

The overall goal of this sub-project is to develop an innovative and integrated EATS for NH_3 conversion systems comprising of low or no precious metal catalysts that are functional at lower temperatures, capable of handling wide variations in exhaust composition, and possessing high solvothermal stability. Our first objective is to development of a system with new materials to deal with NH_3 -slip. The second objective is the perform the design and characterization of new catalyst materials for coupled N_2O decomposition and NO_x reduction in conventional as well as MW-stimulated EATS. The third overarching objective is the development of new spectroscopic setups for exhaust gas component analysis and reactive MD simulations for operando modeling of reaction intermediates that are relevant to the first two objectives.

Work Program

To achieve the first objective, we will identify and characterize promising catalysts for NH_3 reforming. Recent work on bimetallic Fe/Ni- or Co/Ni-compounds have demonstrated comparable performance to Ru and Pd-based NH_3 reforming, and thus offer good starting points for developing a noble-metal-free system [273]. We will also explore the possibility of MW-driven NH_3

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dehydration to produce H_2 in situ. We will develop systems to harness the residual heat from the subsequent oxidation of this H_2 , which can be used for raising the temperature of N_2O decomposition. The use of this H_2 for H_2 -SCR will also be investigated.

In parallel, we will characterize NH_3 storage materials to enable an innovative circular capture and release process. Various material classes such as metal-halides and Metal-Organic-Frameworks (MOF) will be explored for their NH_3 storage capacity, including zeolites [202] from our previous work. Going beyond thermally triggered release of stored NH_3 , we will build upon our previous work [203] and develop a novel strategy of using MW excitation for triggering NH_3 release more rapidly and energy-efficiently. The research on the MW-induced release will generate strong synergies with work on microwave-enabled integrated carbon capture and conversion (ICCC), which is part of SRA-TCP.

For coupled De NO_x -SCR and N_2O decomposition, we will develop transition metal-promoted zeolite catalysts. These catalysts will be tested in conventional EATS test benches characterizing their performance under technologically relevant conditions. Going beyond the state of the art, we will also develop a novel EATS that can enable MW-stimulated non-equilibrium conditions on the catalysts that are adaptive to the combustion system's stoichiometry and emissions. Furthermore, we will develop the corresponding test benches to enable cyclic heated spatial zones on the catalyst material to achieve a constant N_2O decomposition. At the material scale, we will identify promising catalysts that can be readily activated under MW irradiation to generate O or N defects in oxides or nitrides, respectively, and thereby enable the splitting of N_2O . These efforts will be complemented by non-equilibrium MD simulations under the effect of finite electric fields [274], which will help estimate the dielectric losses and surface reactivity of potential MW-active materials. The simulations will also consider dopant and vacancy effects, which will ultimately influence the reactivity. Further, we will connect material properties to their functionality by using non-parametric methods like Symbolic Regression or Compressed Sensing, which can yield rapidly calculable descriptors for screening new materials without needing expensive MD simulations.

These efforts will be complimented by spectroscopic operando monitoring of reaction intermediates and products at the catalysts' surfaces using in-situ DRIFTS, impedance spectroscopy, and mass spectrometry for accurate quantification of the various emissions. To achieve these at scale, we will build an exhaust gas analytic setup for a non-target analysis of carbon-free exhaust-gas components. To build a precise understanding of the complex interplay between catalysts, oxide supports, and reaction conditions, we will use the recently pioneered modified ESM method [275], and analyze the catalyst's stability versus its activity. Going beyond 0 K first-principles calculations, we will simulate the operando interfacial structures and catalytic events using reactive and ML-derived interatomic potentials. These efforts will enable an exhaustive as well as accurate accounting of the effects of H_2O , NO_2 , O_2 , and NH_3 in the exhaust streams.

4.5.2.4 Proposed Staff and Funding of SRA-AFU

Table 4.5.2.1: Proposed Staff in SRA-AFU

Staff category	2026	2027	2028	2029	2030	2031	2032
	Number of persons						
Postdoctoral researchers	3	3	3	3	3	3	3
Doctoral researchers	12	12	12	12	12	12	12

Table 4.5.2.2: Funding Request for SRA-AFU

Funding category	2026	2027	2028	2029	2030	2031	2032
	Totals per year in thousand euros						
Staff (Total for 4.5.2)	1121	1143	1166	1189	1213	1237	1262
Direct project costs (excluding staff)	335	300	180	180	180	180	180
Total instrumentation < €150,000	160	175	0	100	0	0	0
Total instrumentation > €150,000	0	170	150	0	0	0	0
SOFC single cell test bench		170					
HD-cylinder head			150				

Instrumentation below 150 k€

To investigate the interaction of NH_3 and H_2 with respect to both H_2 -bubbling in liquid NH_3 and degassing of solved H_2 in NH_3 inside injector nozzles, a dynamic phase transition evaluation rig using a transparent nozzle is required (60 k€). To deliver tailored NH_3 - H_2 - N_2 mixtures, the investigation of catalytic NH_3 decomposition either prior or integrated into the ammonia combustion engine requires an online analysis system of ammonia decomposition (100 k€). For the optical investigation of the NH_3 combustion process, the optical single-cylinder engine from FSC has to be adapted (100 k€) and an IR camera incl. optical equipment is required (75 k€). The investigations of DAFCs with respect to the volumetric flow field measurements of narrow channels and channel structures, the experimental analysis of the interaction of gas bubbles and fluid flow in narrow channels, and the investigation of rough surface structures in narrow channels require a micro PIV system including a microscope (100 k€).

Instrumentation above 150 k€

To investigate ammonia fuel cells, a preexisting flex-fuel, reversible direct liquid SOFC single cell test bench has to be upgraded, including the vaporizer, the power source, the external reformer, and the electrochemical impedance spectroscopy (170 k€). For the thermodynamic development of the NH_3 combustion process, a new cylinder head for the thermodynamic single-cylinder engine is required (150 k€).

4.5.3 SRA "Concatenated Synthetic Pathways" (SRA-CSP)

PIs: Palkovits, von der Aßen, Blank, Eichel, Herres-Pawlis, Jupke, Klankermayer, Lauterbach, Leitner, Mayrhofer, Rother, Schoenebeck, Waldvogel, Wessling, Zobel; ARs: Bolm, Wiegand

This SRA aims to develop the catalytic toolbox for concatenated synthetic pathways necessary to generate a flexible bio-hybrid platform of molecular building blocks that can be integrated into resilient material cycles [57]. On the molecular level, **adapted catalytic systems** are designed to enable versatile methods of bio-hybrid synthesis allowing the sustainable formation of C–C, C–H, C–O, and C–N bonds **integrating renewable energy as well as renewable carbon and nitrogen sources**.

Traditionally, each step in the intended sequence of transformations is optimized individually including catalyst performance, reactor configuration, and down-stream processing. In such a reductionist approach, different catalytic technologies are often perceived to compete for the best performance in a specific step, but the resulting sequence of transformations ultimately compromises on lower levels of efficiency due to incompatibilities in the transfer between them. Instead, **concatenated synthetic pathways take a system's approach**. They target **integrating both catalytic transformations as well as unit operations** on the levels of catalyst, reactor, and process. Therein, the individual catalytic disciplines do not compete with each other but are fundamentally equivalent solutions in the overall system aiming at optimizing the overall energy and material balance through **appropriate levels of integration** (Figure 17). Accordingly, methodologies for implementing concatenated synthetic pathways on the different levels reaching from bio-hybrid synthetic pathways reaching from bio-hybrid synthetic pathways over interconnected catalytic systems to integrated reactor concepts are in focus of this SRA.

Strategy and Structure of SRA

Concatenated synthetic pathways are considered on different length scales. At the molecular level, we focus on catalytic transformations for **bio-hybrid syntheses** (Sub-SRA CSP-1) that allow accessing the same products from different future carbon and nitrogen resources and via different catalytic pathways or that provide chemical compounds structurally composed of motifs from different future carbon sources. Within reaction cascades, **interconnected catalytic systems** (Sub-SRA CSP-2) enable an optimum combination of catalytic transformations using catalysts of various origin (bio-/chemo-/electrocatalysts) and separations along a value path towards maximum resource efficiency at minimum energy needs and operational costs. Ultimately, catalytic transformations together with the optimum separation technology are combined in **integrated reactor systems** (Sub-SRA CSP-3) to provide the most desirable process concept.

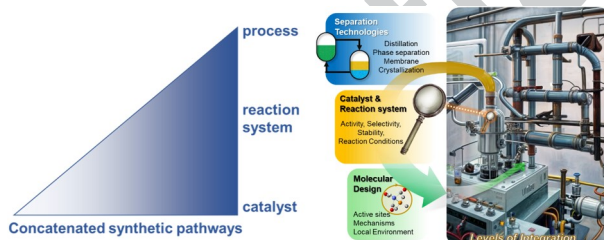


Figure 17: Holistic design of concatenated synthetic pathways considering the various options on the levels of catalyst, reaction system, and reactor and process design for an overall optimum.

4.5.3.1 Bio-hybrid Synthesis

Detailed investigations of future scenarios indicate that only the **integrated and flexible use of all available alternative future carbon and nitrogen sources** will enable the chemical conversion of renewable energies on a scale relevant to the path to a **resilient mobility and chemical sector**. This integrative use provides bio-hybrid fuels and chemicals that not only have the potential to meet the high demand for renewable liquid fuels, but also offer a greater variety of possible molecular structures to produce important chemicals for a sustainable society. Key are selective catalysts facilitating tailored access to the molecular motifs of the bio-hybrid platform based on versatile raw materials. Catalyst development proceeds iteratively by combining forefront experimental and computation methodologies covering high-throughput synthesis and screening, operando analytics and data sciences.

Current State of Research and Previous Work

Prior studies within the clusters of excellence Tailor-Made Fuels from Biomass (TMFB) and FSC allowed establishing a broad toolbox of catalysts for valorizing lignocellulosic biomass as well as CO₂. In these feedstocks, in contrast to fossil fuels, carbon is present in high oxidation state requiring selective defunctionalisation or reduction. For CO₂, catalyst systems providing access to all relevant levels of carbon oxidation state could be developed by rational catalyst design. This includes new strategies for the reduction of CO₂ to CO, formic acid, as well as methanol with molecular or solid chemocatalysts as well as electrocatalysts. Major breakthroughs in the use of catalysts based on earth abundant 3d metals have been achieved. A nickel-based catalyst comprising a Triphos-ligand was shown to exhibit outstanding activity for formic acid formation [58]. The first catalytic system allowing direct hydrogenation of CO₂ to methanol based on manganese as active metal was designed based on a combination of experimental and computational methods. Utilising ligand structures as building blocks of materials, solid molecular catalysts composed of mono- and bidentate phosphines, pyridine, and triazine motifs and lately even tert-pyridine structures could be derived. Their use in both continuous liquid and gas-phase catalysis was demonstrated. Herein, the dynamics of palladium single-atoms on graphitic carbon nitride were studied during ethylene hydrogenation and H₂-D₂ exchange. By employing aberration-corrected STEM, XPS, and XAS, metal clusters, rather than single-atoms were confirmed as active species [59]. In contrast to formic acid and methanol as target products, the direct hydrogenation of CO₂ to formaldehyde still presents a largely unsolved challenge. Research from FSC has made important contributions in this area by demonstrating the possibility to intercept the CO₂ hydrogenation on the formaldehyde level by *in situ* conversion into fuel and chemical targets. The concept was systematically established for the catalytic synthesis of linear and cyclic acetates as bio-hybrid fuels by valorizing various biogenic alcohols or plastic waste [60]. First concatenated bio- and chemo-catalytic steps were successfully demonstrated by interdisciplinary collaboration of the FSC teams [61]. Though, many challenges remain. Even with regard to the selective hydrogenation of CO and CO₂ to higher alcohols, methodologies to derive C₂₊ alcohols remain rare. In an innovative approach,

Fischer-Tropsch synthesis to olefines was combined with reductive hydroformylation [62]. A heterogeneous cobalt catalyst with high olefine selectivity could be integrated in tandem with thermostable molecular cobalt reductive hydroformylation catalysts to produce a slurry-phase direct conversion of syngas to higher alcohols. For carboxylic acids beyond formic acid, a synthetic pathway to acetic acid via the formal isomerisation of methyl formate combining the two C1 products formic acid and methanol was established [63]. Applying concatenated reaction principles, *in situ* catalytic generation of CO coupled with catalytic carbonylation of biogenic alcohols was shown to open access to novel bio-hybrid pathways to aliphatic carboxylic acids. Inserting CO₂ by carboxylation into nonactivated C-H bonds provides an attractive yet hitherto largely elusive catalytic transformation. Based on a computationally predicted Pd(II) complex, such a reaction could be realized using simple and nonactivated arenes and allowed synthesis of veratric acid, an intermediate for pharmaceutical production, from CO₂ and veratrole.

Valorising bio-catalysis, microbial CO₂ assimilation and conversion to succinic acid was investigated by stoichiometric metabolic modeling based on physiological and process data. Different process variants for the conversion of C1 carbon compounds were studied [64]. Aiming for itaconate production, 72 different Ustilaginaceae strains from 36 species were investigated for their ability to (co-) consume the CO₂-derived substrates acetate and formate. *Ustilago maydis* and *Ustilago rabenhorstiana* were identified as promising candidates for acetate metabolization, whereas *Ustilago cynodontis* was identified as production host using formate as co-substrate enhancing itaconate production. This proof-of-principle study clearly highlighted the potential of biocatalysts for carbon-neutral itaconate production. [65]

Electrocatalytic carbon dioxide reduction (CO₂RR) has also significantly evolved in recent years. For industrially relevant current densities at high selectivity, an integrated catalyst and reactor design proved essential. Due to the important role of the local environment at the electrodes, its assessment under true catalytic conditions is highly relevant. Multinuclear *in operando* nuclear magnetic resonance (NMR) techniques were applied to CO₂RR in aqueous NaHCO₃ or KHCO₃ over silver electrodes. ¹³C and ²³Na NMR studies confirmed a slowing of the dynamic equilibrium of the electrolyte salt in solution, which is present in the form of ion pairs and free ions, with increasingly negative potential, affecting the CO₂ resupply rate from the electrolyte. Substantiated by relaxation measurements, stable ion pairs in solution were proposed to catalyze the bicarbonate dehydration reaction [66]. Electrochemical real-time mass spectrometry (EC-RTMS) provides real-time information on transients occurring at dynamic interfaces. Applied to CO₂RR during potential step or sweep experiments on pristine and *in situ* anodized copper showed enhanced formation of several C₂₊ products over C1 products directly after copper anodization, with unprecedented temporal resolution. This creates exciting opportunities for resolving processes at short timescales and under dynamic operation. [66]

Regarding biomass, a broad set of chemo- and biocatalysts had already been developed within the CoE TMFB enabling the conversion of lignocellulosic biomass to a variety of intermediates or products. In FSC, the catalytic toolbox could be significantly broadened by utilising electrocatalytic biomass valorization. Kolbe electrolysis was explored to transform biogenic carboxylic

acids to monomers and fuels [67], e.g., by electrochemical cross-coupling of biogenic di-acids allowing to flexibly tailor the fuel structures. As overarching concept, anodic transformation at lower potentials compared to oxygen evolution reaction were explored for enabling electrocatalytic hydrogen formation at lower cell potentials accompanied by anodic formation of valuable products. An example comprehends glycerol electrooxidation, where bimetallic PtCu electrocatalysts enabled superior selectivity to C₃ products which proved important in economic analysis of this technology [68]. Regarding electrocatalyst prediction, comprehensive material characterization highlighted covalency as electronic descriptor able to rationalize catalytic activity of transition metal perovskites in both oxygen evolution reaction (OER) and glycerol electro-oxidation as well as chemocatalytic NO reduction and N₂O decomposition [69].

FSC² PIs also made first steps into integrating nitrogen functionalities in the valorization of renewable feedstocks. Comprehensive LCA and techno-economic analysis of the heterogeneously catalyzed amidation of succinic acid to the monomer N-vinyl-2-pyrrolidone (NVP) was carried out. Indeed, LCA projected bio-based NVP production to reduce global warming impacts by 25–53% compared to today's fossil alternative [70]. Combining microbial cell factories, enzyme cascades, and chemocatalysis, hydroxy ketones and amino alcohols could be gained in high yield and excellent selectivity from second generation feedstocks. In the atom- and step efficient process, downstream processing was directly integrated. A flexible catalyst platform was demonstrated for the one-pot synthesis of valuable allylamines and alkylamines from amines, formaldehyde, and terminal alkynes. The multifunctional catalytic system comprehends a silica support on which are jointly assembled ruthenium nanoparticles and covalently functionalized copper N-heterocyclic carbene (NHC) complexes. Detailed investigations confirmed that the immobilized molecular Cu(I)-NHC complex is responsible for the atom-efficient A₃ coupling of amines, formaldehyde, and terminal alkynes, while selective hydrogenation of the resulting propargyl amines is catalyzed by Ru nanoparticles. This flexible design platform opens the way to the development of multifunctional catalytic systems capable of performing complex reaction sequences in one pot.

Objectives

The objectives comprehend (i) creating an adaptive and integrated access to new bio-hybrid structures for sustainable chemical conversion processes, (ii) developing the therefore necessary bio-, chemo- and electrocatalysts with tailored active sites for a flexible transformation of various carbon and nitrogen sources using renewable energy; (iii) accelerating catalyst development and reaction pathway design by mechanistical insights, parallelized and automated screening and data-driven optimization, ultimately aiming for prediction.

Work Program

With the aim of providing a catalytic toolbox that offers a flexible biohybrid platform of molecular building blocks that can be integrated into resilient material cycles, methodological advances are sought that enable the sustainable formation of C–C, C–H, C–O, and C–N bonds based on

all future available carbon sources and nitrogen (Figure 18). Concatenated bio-, chemo-, and electrocatalytic pathways for bio-hybrid fuels and chemicals are enabled by integrated catalyst development, complemented by the tailored interplay of experimental methods, analytical techniques, and modeling approaches, ultimately leading to the establishment of digital tools for the interlinked catalyst-process design and structure-function prediction.

Especially the **formaldehyde platform** provides tremendous potential. Building upon the previously demonstrated access to compounds in the formaldehyde oxidation state, direct catalytic transformations e.g. by CO₂ reduction to formaldehyde and derivatives will be targeted. Research objectives comprehend **methodologies to provide free formaldehyde** by chemo-, bio- [71], and electrocatalysis (Klankermayer, Leitner, Rother, Wessling). Formaldehyde corresponds to the same formal reduction level as carbohydrates and hence presents an **attractive C-source for microbial transformations** (Blank). Inspired by the cluster's previous success regarding **in situ chemical transformation to formaldehyde derivatives**, the synthesis of linear and cyclic acetals will be extended and further developed providing input towards translation (Blank, Klankermayer, Leitner, Palkovits, Rother). Novel concatenated pathways will be explored exploiting the intrinsic reactivity of the formaldehyde molecule in particular towards condensation reactions. As demonstrated in FSC most recently for the selective β -methylation of alcohols [72], the platform will serve as a starting point for new catalytic approaches towards **C-C bond formation** (Klankermayer, Leitner, W3 Digital Chemistry).

Tailored catalytic transformations using the **formaldehyde platform towards the synthesis of nitrogen containing compounds** will be also in focus. This includes selective synthesis of amins in analogy to the acetals and N-methylation reactions based on CO₂ instead of formaldehyde. Beyond formaldehyde, further approaches of **C-C and C-N bond formation** present major focus points of FSC² research. In this context, innovative homologation concepts for C1 building blocks of all oxidation steps play a major role. Examples comprehend chemocatalytic approaches towards higher alcohols synthesis as well as C2+ products in electrocatalytic CO₂ valorization. Also, novel strategies for nitrogen insertion are essential, to transform e.g. biogenic acids into the related amines. Exemplarily, formate will be enzymatically converted to formaldehyde and subsequently directly upgraded via C-C bond and C-N bond formation. In these multi-enzyme catalysed processes, mono- and dihydroxy ketones and amino alcohols are formed in a selective manner, which are platform chemicals for further diversification with enzymes or chemical catalysts in one-pot or multi-pot reaction systems. Building upon a mechanochemical activation of Mg and subsequent reaction of the *in-situ*-generated organometallic reagent with CO₂ [73], N₂ activation by Ti will be studied. Ultimately, novel approaches to N₂ fixation and a

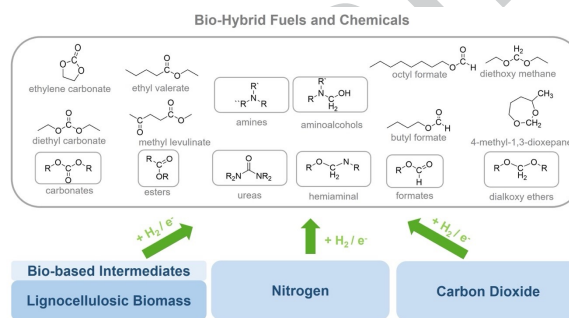


Figure 18: Catalytic toolbox for flexible access to bio-hybrid fuels and chemicals enabled by the sustainable formation of C-C, C-H, C-O, and C-N bonds.

direct activation of both N_2 and CO_2 will be explored in FSC² (Bolm, Wiegand, Zobel).

Tools of automated catalyst synthesis, high-throughput screening, operando analytics, and AI-added data evaluation will be broadly valorized to accelerate development and ultimately catalyst prediction. As example Schoenebeck group showcased the potential of ML methods to predict previously unknown dinuclear Pd catalysts [74–79]. In FSC², this approach will be advanced further and applied to exploit catalysts enabling C–C and C–N bond formation. In the next step, catalyst prediction will be coupled with automatized catalyst synthesis platforms as key step for fully integrated workflows [80–82].

Accordingly, methodologies for parallelized and high-throughput testing together with the necessary data management and evaluation as already developed e.g. in electrocatalysis [83–85], will be extended to the other catalysis disciplines (Klankermayer, Palkovits, W2 Catalyst Development, W3 Digital Chemistry). Operando-analytics present a crucial element of knowledge-based accelerated catalyst design. The development of tools reaching from accelerated over parallelized to automated testing and investigation under operando conditions together with the necessary methodologies for data evaluation, modeling, and prediction of catalysts and reaction systems presents a strategic element in FSC². On the one hand, FSC² PIs will integrate these methods into their work processes and a junior research group on parallel catalyst synthesis and testing will be established. On the other hand, a new professorship will be established at the interface of chemistry, mechanical engineering, and computer science (W3 Digital Chemistry), to enable developments in this fast-growing area of cutting-edge research that shape the international state of research.

4.5.3.2 Interconnected Catalytic Concepts

To leverage the full potential of novel, sustainable, effective processes for bio-hybrid fuels or chemicals, the concept of interconnected catalytic systems is explored. Therein, catalytic transformations by bio-, chemo- or electrocatalysts are closely integrated to efficiently reduce synthesis steps and/or to switch from the classic approach of using one type of catalyst for a process to a combination of catalysts. In this way, advantages of catalysts from different disciplines are combined aiming for maximum resource and energy efficiency. Accompanied by an integrated holistic design of efficient separation technologies, an overall optimum for transformation sequences will be derived. Due to the broad expertise of the partners, aqueous, organic and multiphase systems as well as all types of reactor designs (see Sub-SRA CSP-3) are available for modular and flexible combinations. The outstanding element of this FSC² approach is the techno-economic overall balancing of the process including the catalytic reaction sequence as well as required separation steps.

Current State of Research and Previous Work

While the fundamental principle of catalysis with biocatalysts, chemo- or electrocatalysts is universal, the different catalysis disciplines come with their unique advantages and challenges. To valorize the full potential of the complementary advantages of catalysis disciplines, their intimate

integration along transformations paths by compatible, smart reaction systems is essential. This can be achieved by compartmentalizing catalyst types in separate phases, e.g. in liquid/liquid multiphase systems, or by adapting them to alternative solvents or multiphase reaction systems. Prior studies have already highlighted the potential of bridging different catalytic functionalities and disciplines as well as closely integrating separation technologies in the development.

Short chain diols, such as 2,3-butanediol, present interesting intermediates for alternative low carbon, low-emission fuels, and bio-hybrid chemicals [58]. They can directly be produced from biomass with *Enterobacter* or *Klebsiella* strains, but the energy-intensive separation of this hydrophilic, high-boiling compound from an aqueous reaction system via distillation is unfavorable [86]. Accordingly, novel porous framework materials were developed enabling selective separation even of challenging mixtures such as trans-1,2-diols over cis-1,2-diols as well as a direct removal of diols from fermentation broths [87, 88]. In an alternative approach, whole-cell and enzyme catalysis were combined. A yeast-based acetaldehyde production with in situ gas stripping and capture was used [89]. Due to the high vapor pressure of acetaldehyde, it evaporates from the bioreactor and thus “distills itself”. A two-step enzymatic cascade allowed converting bio-based acetaldehydes to vicinal diols in a micro-aqueous environment. As the 2,3-butanediol is produced in an organic monophase, downstream processing is extremely facilitated [90]. Subsequently combined with chemocatalytic CO₂ incorporation in the formaldehyde oxidation state, cyclic and linear acetals become accessible broadening the available bio-hybrid chemical platform [6]. This concatenated synthetic pathway clearly exemplifies the potential of the integrated development of alternative production routes to minimize the effort for product separation and to make sustainable production paths more sustainable and competitive.

Recent advances for chemocatalysis in biological media [91] and biocatalysis in unconventional media [92] confirm that it is possible to run the respective catalysts in media other than classically applied. The following example from the FSC impressively demonstrate the combination of catalysts in one pot and that applying e.g. green organic solvents, even offers advantages for catalysts of different origin: Taking the biggest biotechnological example, the production of bioethanol is fast with $> 1 \text{ g L}^{-1} \text{ h}^{-1}$, efficient with $> 90 \%$ theoretical yield, and the product can accumulate up to 150 g L^{-1} [93]. Still, starting from glucose even at 100 % theoretical yield, every third carbon atom is lost as CO₂ in the process due to reaction enthalpy reasons. For a reaction to be efficient, not only high yields are needed, but as few atoms as possible should be wasted [94,95]. To increase the atom economy – in this case for valuable carbon – of bioethanol fermentations, CO₂ might be directly uptaken. Within the FSC, Guntermann and Mengers et al. explored this by converting the microbial-produced waste-CO₂ in a 1-step, 1-pot approach [96]. Molecular ruthenium complexes are known to catalyze H₂-driven CO₂ reduction to formate, a non-volatile, non-toxic, valuable animal and microbial co-feed under mild conditions. Separating the catalysts with contradictory demands either timely or spatially simplifies the method development, but an integrated system can ultimately outperform complex connected reactors due to less needed separation steps. After conflating the reaction conditions, the bioethanol fermentation was carried out in a high-pressure reactor under 120 bar of H₂ pressure simultaneously coupled with a Ru-catalyst residing in a tetradecane phase converting CO₂ and H₂ to

formate. Ultimately, over 26 % of the nascent greenhouse gas (GHG) were converted to formate. Simple separating the fermentation broth from the non-polar organic phase allowed for effective recycling of the precious organometallic catalyst. With a global bioethanol CO₂ output of 50 Mt a⁻¹, although minuscule compared to 31,900 Mt a⁻¹ from fossil fuels [97], could mean a CO₂-negative production of 13 Mt a⁻¹ formic acid, if this reaction concept would be globally applied. And the concept can be pushed even further. Both formate and ethanol can be converted enzymatically to larger molecules of higher value, like ethyl formate, in the same 1-step, 1-pot process, using the complete spectrum of catalysis [98].

Objectives

The objectives comprehend (i) combining different catalyst types into concatenated reaction sequences. Therefore, compatible reaction systems are designed, (ii) directly integrating the development of separation steps into the design of concatenated transformations (iii) to achieve pathways with lowest possible energy demands and environmental footprint by overall process balancing.

Work Program

Important aims are [integrated processes combining challenges in catalysis and product separation](#). Conventionally, sequential conversion and separation along a reaction sequence involves incorporating separation steps – usually energy consuming distillation – after each reaction step to purify the intermediate to the required purity of the following step. While providing flexible process operation, this approach often results in energy intensive separation tasks. To address this, [energy efficient separation techniques](#) for the mostly polar products from polar solvents will be explored including extraction, adsorption, or membranes. To this end, experimental investigation as well as modelling of binding and interaction mechanisms in novel reactive separation systems consisting of tailored solvents (e.g., deep eutectic solvents) and adsorbents (e.g., functionalized polymers) will be performed (Jupke, Palkovits) as well as characterization of novel membranes (Wessling). Specific examples include reactive extraction to separate carboxylic acids or amines from reaction mixtures. In addition, adsorptive techniques for the separation of diols from aqueous solutions are being developed. Moreover, integrating transformation and separation is targeted. To effectively evaluate separation strategies, early-stage overall process design and optimization will be applied in close cooperation with the fuel and chemical design approach (Sub-SRA RACS-1). A major challenge is that at an early stage of development, there is only limited experimental data available. FSC² will overcome this challenge by combining hybrid mechanistic- & data-driven models, experimental data, and the use of uncertainty quantification, thus enabling rational identification of the most promising options at the process level (Jupke, Mitsos). By identifying key factors and bottlenecks in an early stage of development, the full potential of concatenated synthetic pathways can be valorized.

On the reaction level, the individual conversions and their respective reaction conditions are traditionally optimized individually hampering integration along the reaction cascade. In con-

catenated reaction systems, reaction sequences involving different catalytic transformations proceed within a tailored reaction system enabling close integration. We therefore focus on **smart solvent selection for multiple consecutive conversion steps** with less or even without solvent change facilitating an efficient sequence with less separation effort (Blank, Klankermayer, Jupke, Mitsos, Rother). The challenge of solvent selection arises from the trade-off between different optimization criteria, such as the influence on catalytic performance and energy-efficient separation. Different types of catalysts (bio-, chemo- or electrocatalysts) have different optimal reaction solvents, whereby thermophysical properties play a decisive role for the catalytic activity. In addition, product separation can be facilitated by a smart choice of solvent [204,205]. Systematic solvent selection will be performed by developing new model-based approaches. Determining optimal trade-offs between requirements using model-based or AI-driven approaches depends on knowledge of thermodynamic properties, so the integration of property databases, property prediction calculation methods and experimental data is crucial (Jupke, Leonhard, Mitsos). Ultimately, achieving a balance between catalytic efficiency and separation performance is key to developing sustainable and economically viable chemical processes.

To design truly novel, efficient processes from substrates for sustainable chemical industry with minimal footprint, FSC² will now extend this concept towards further chemical products, blends and fuels in optimally one-pot processes with minimal separation effort. Here, all types of solvent systems, ranging from aqueous or organic monophasic over biphasic towards compartmented reaction systems are considered. They are evaluated with respect to energy and resource consumption as well as environmental performance parameters. A first example highlights the integration of multiple disciplines to derive potent solutions. Here, aliphatic as well as aromatic-aliphatic 2-hydroxy ketones will be synthesized based on microbially produced butanal and aromatic compounds (from second generation feedstocks) ligated with formaldehyde (from CO₂ fixation). From these intermediates, a set of products like diols, dioxolanes and amino alcohols will be accessible by further diversification with enzymes and chemo-catalysts. In sum, by the modular combination of (electro-)chemistry, transformations with microbial cell factories and enzyme cascades, a broad product portfolio based on bio-hybrids is accessible. Automation and model-based predictions will support the optimization of the overall synthesis pathway, including downstream processing. (Klankermayer, Leitner, Palkovits, Herres-Pawlis, Rother, Blank, Lauterbach, Magnus, Jupke, Walther, Heufer)

Efficient coupling to biocatalytic steps is also possible by means of electro-catalysis. Prior studies demonstrated electrochemical reduction of itaconic acid to methylsuccinic acid as well as non-Kolbe electrolysis of 3-Hydroxy decanoic acid (3-HDA) within fermentation broths [206].

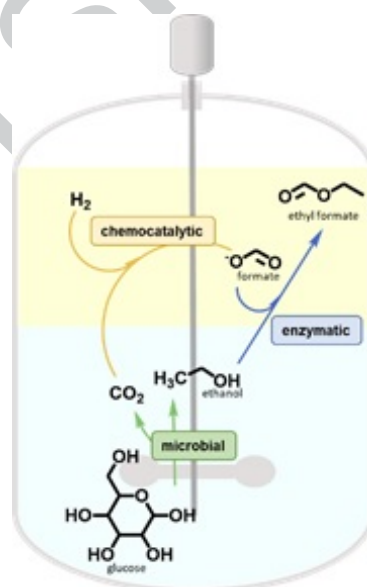


Figure 19: Combination of microbial, chemocatalytic, and enzymatic catalysts for the integrated synthesis of ethyl formate from biomass and CO₂ in a one-pot, two liquid-phase reactor.

Accordingly, current studies on electro-catalytic amination [207, 208] will be extended in FSC² for valorizing carboxylic acids as well as other biocatalytically accessible aldehydes and ketones. Beyond substantial reduction of unit operations and energy requirements, *in operando* integrating electrochemistry and biotechnology is aimed for (Blank, Jupke, Palkovits).

4.5.3.3 Integrated Reactor Devices

The future available carbon and nitrogen sources, which will be converted into bio-hybrid fuels and chemicals by chemo-, bio-, or electro-catalytic conversion steps, result in complex multi-phase reaction mixtures. Moreover, these systems are subject to fluctuating supply of raw materials and renewable energies. Therefore, optimal design and operation of flexible and adaptable multi-phase reactor devices play a pivotal role. To achieve high yields in multi-phase reactors under flexible operation applying the catalytic toolbox from Sub-SRA CSP-1, novel intensified reactor devices and operating concepts will be developed. Our aim is to design and operate adaptive, autonomous, and self-optimizing multi-phase reactors targeting high yield and selectivity under flexible operating conditions. To cope with fluctuating feed streams and energy supplies, we will consider modular and scalable reactor architectures that can be numbered up and cascaded. We will break the envisaged modular units down into smaller repeating sub-units, such as tubular or 3D printed flow devices. Tailor-made approaches of experimental analysis and simulative methods are developed that enable us to understand the complex interplay of underlying phenomena such as reaction and mass transfer kinetics, phase equilibria as well as interfacial and fluid dynamics, especially at reaction conditions. To this end, high-resolution measurement methods and *operando* technologies (e.g., 2D Raman, in-line infrared, Raman or NMR spectroscopy) are used. Fundamental phenomena are investigated on the smallest scale and control mechanisms are explored. Based on this understanding, the goal is to operate self-optimizing autonomous multi-phase reactors under flexible operating conditions using monitoring techniques as well as model-based and data-driven control techniques.

Current State of Research and Previous Work

In the FSC, we successfully designed and operated several novel reactor devices for the production of bio-hybrid fuels, like multi-phase tubular reactors or (electrochemical) reactors for emulsions or suspensions. We also targeted the integration of conversion and product separation in one device by *in situ* product removal to suppress equilibrium limitations, by-product formation, and product inhibition. For example, we managed the biochemical production of methyl ketones where the product is *in situ* extracted in a second liquid phase to prevent product inhibition and emulsion formation in a newly developed multi-phase loop reactor [99].

Further, *in situ* product removal can be leveraged so that the chemical reaction acts as the product sink for a biotransformation and vice versa. We realized the homogeneously catalyzed chemical conversion of H₂ and CO₂ to formic acid and subsequent extraction into an aqueous phase, where formic acid is converted into itaconic acid by biotransformation. Finally, the CO₂ release of the microbes is used as substrate for the chemical conversion [100].

Liquid phase chemical reactions also benefit from applying in situ product removal and merging reaction as well as separation in a multi-phase reactor. This involves introducing a second liquid phase. In the case of gaseous reactants such as H_2 and CO_2 , complex three-phase vapor-liquid-liquid systems occur in which flow pattern and mass transfer from the gaseous into the liquid phases must be considered. We were able to demonstrate that in situ product removal reduces side reactions and overcomes equilibrium limitations to achieve higher yields. For instance, an integrated reaction network consisting of a biphasic homogeneously catalyzed hydrogenation of CO_2 to formic acid was realized [101].

Furthermore, we developed a new biphasic reactor device for the conversion of fructose via 5-hydroxymethylfurfural (5-HMF) to furandicarboxylic acid (FDCA), resulting in the highest 5-HMF yield published to date [102].

Based on the measurement of phase equilibria as well as reaction and mass transfer kinetics at reaction conditions, we developed a customized simulation model. Using this model, we realized the optimal design of a continuously operated biphasic tubular reactor in which 5-HMF is extracted in countercurrent flow from the reaction phase to prevent by-product formation [205]. The process was further intensified by a consecutive electrochemical conversion of 5-HMF to FDCA. By directly feeding the organic 5-HMF from chemical conversion to a biphasic electrochemical reactor, the new integrated process eliminates the need for an intermediate purification step (Figure 20) [104].

A comparable approach was realized for the direct utilization of a fermentation product in an electrochemical reactor. First, we electrochemically reduced acetoin to 2-butanone directly within the fermentation broth. In a second step, we were able to increase the efficiency of the electrochemical reduction reaction through the adaption of the fermentation to a minimal media fermentation, which reduced parasitic side reactions in the electrochemical flow-cell [105].

New 3D printed tubular electrodes enable modular electrochemical reactor concepts with high surface to volume ratios. We demonstrated that additive manufacturing, like selective laser melting, offers high flexibility and control in the manufacturing of tubular gas diffusion electrodes in terms of porosity and pore size distribution [106]. In the next step, several tubular

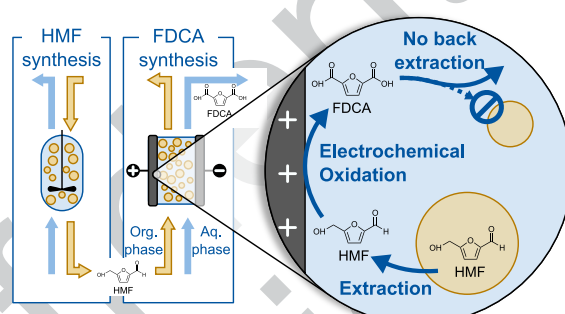


Figure 20: Integrated conversion of fructose to FDCA in a biphasic systems comprising chemical and electrochemical conversion.

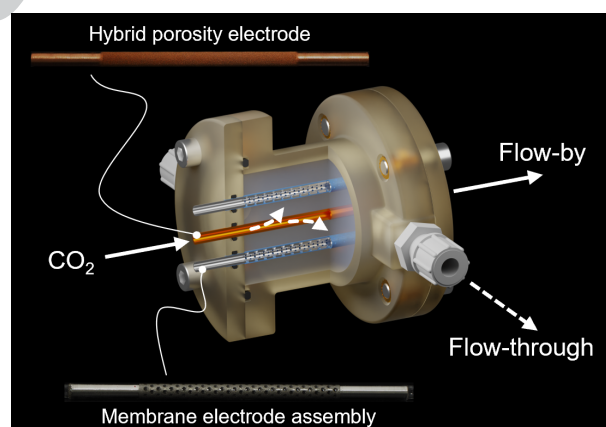


Figure 21: Flow reactor for 3D printed tubular gas diffusion electrode with tailored porosity.

electrodes were integrated into one reactor device, which enables swift scale-up via numbering-up (Figure 21) [107]. We also exploited the high degree of freedom in design by 3D printing triply periodic minimal surfaces (TPMS) entities [108] and integrating two functions into the electrode domain: high active surface area and enhanced mass transfer [211]. Finally, we developed a new way to improve electrochemical reactors by using the dynamic extension of electrochemically active surface area via flow electrodes or slurry electrodes [110].

Objectives

The objectives comprehend (i) the development of scalable and modular reactor devices which allow bio-hybrid fuel and chemical production, (ii) integrated reaction and separation for intensified processes and (iii) autonomous and self-optimizing operating concepts enabling high yields and selectivity over a wide range of operating conditions.

Work Program

Building on the previous work, the aim in FSC² is to develop the necessary fundamental knowledge for the [design and operation of self-optimizing, autonomous multi-phase reactors](#) under flexible operating conditions. We strive to design reactors that facilitate [stimuli-responsive activation of catalysts and local reaction control](#) by leveraging advanced materials processing to trigger via electrical, thermal, or pH-dependent actors. Additionally, we not only design reactors to cope with fluctuating input streams, but we aim to dynamically control and pulse current, flow, temperature, wettability (and more) to optimize yields and selectivity. These reactors will be self-optimizing entities, for which we apply monitoring techniques and employ [model-based design and control strategies](#). In the lab, the reactors will not only be equipped with online analytics, but also visual observation to feed information into control tools [276].

The complexity of multi-phase reaction systems results from the intricate interplay of different phenomena on micro-, meso-, and macroscale, rendering a significant challenge for modeling and control. For this purpose, underlying phenomena such as reaction and mass transfer kinetics, phase equilibria as well as interfacial and fluid dynamics, especially under reaction conditions, need to be understood. Hence, there is a clear imperative to develop a systematic approach for the design, operation, optimization, and scaling of multi-phase reaction devices. Within these devices, products are formed via bio-, chemo- or electrocatalysis, which can be intensified via in situ product removal. In situ product removal means separation of target molecules at their point of origin to suppress or minimize equilibrium limitations (Palkovits, Klankermayer, Leitner), product inhibition (Blank, Rother, Magnus, Lauterbach), and undesirable by-product formation (Jupke, Wessling). This integrated approach improves operational efficiency (yield, selectivity, space-time-yield) and ensures optimal performance.

Two reactor concepts are pursued to cover underlying phenomena: (i) a multi-phase electrochemical reactor (Wessling) (Figure 22), and (ii) a multi-phase tubular reactor with chemo-, or bio-catalytic conversion (Klankermayer, Jupke, Rother), see Figure 23. These concepts will serve as joint platforms to promote the integrated research. Both devices have the common

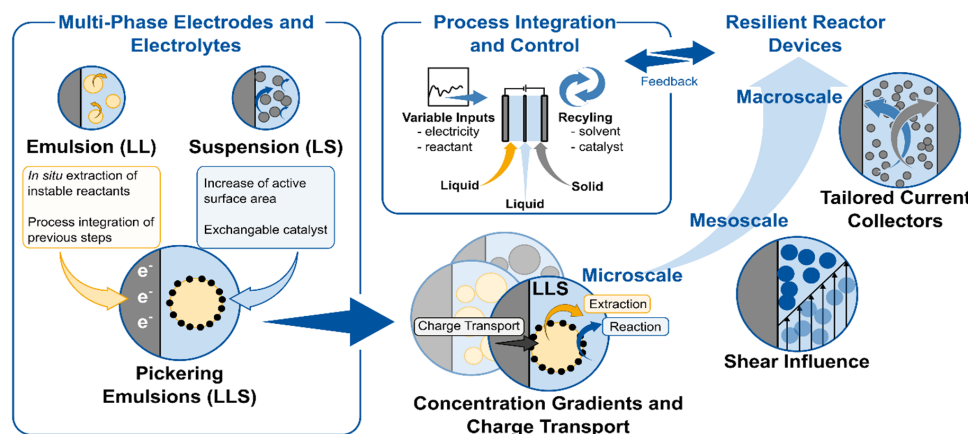


Figure 22: Scale based approach for multi-phase electrochemical systems.

feature of precisely tuned multi-phase flows and tailor-made catalysts inside one device.

On the **microscale**, the aim is to understand the reaction pathways and equilibria. In addition, a comprehensive knowledge of the complex interactions between reaction kinetics and mass transfer will be investigated, considering thermodynamic phase equilibrium and local fluid dynamics. To address this, interfacial mass transport and reaction kinetics will be studied using a 2D Raman technique to further develop reactive computational fluid dynamics (Jupke, Pitsch, Wessling). Additionally, we aim to study charge transfer and faradaic reactions in suspension electrodes, also known as flow-through electrodes, which extend the electrochemically active surface through the addition of conductive particles (Wessling). Moreover, we will extend the concept of suspension electrodes to Pickering emulsions, in which the second liquid phase enables in situ product removal or efficient reactant supply to the catalytic surface. Figure 22 shows the multi-scale approach applied to electrochemical multi-phase reactors. Electrochemical interfaces and their reactions can be significantly enhanced by applying pulsed electrolysis (Mayrhofer, Wessling).

To derive crucial experimental data of the underlying phenomena, we will conduct measurements using sophisticated analytic techniques, such as Raman, infrared, and fluorescence lifetime spectroscopy, distribution of relaxation times, under relevant process conditions, which best approximate the operating space. Occurring phenomena need to be understood and interpreted with the help of models in order to draw appropriate conclusions for the subsequent reactor design and operation. For a better understanding of the underlying physicochemical effects, rigorous mechanistic models will be developed and validated.

On the **mesoscale**, our research methodology aims to derive suitable reactor models to couple previously measured microscale effects with mesoscale phenomena (e.g., swarm behavior, local dispersed phase hold-up, total mass transfer area). For mechanistic modeling, we will use differential algebraic equations to dynamically model the complex interplay of multi-phase phenomena, e.g., reaction and mass transfer kinetics, phase equilibria as well as interfacial and fluid dynamics. However, the identification of physical phenomena sensitive to variations in e.g. feed or power supply is critical to guide operational decisions to mitigate potential prob-

lems. Therefore, the modeling framework incorporates detailed sub-models to account for the multi-phase phenomena enabling the prediction of the complex flow regime in the reactor considering fluctuations. In order to track dynamic multi-phase phenomena, the reactor will be equipped with sensors, such as high-speed cameras for online droplet size and motion detection [111]. The experimental data from the sensors will finally be used for online parametrization of the sub-models enabling performance and condition monitoring. Figure 23 illustrates the bridge across the scale for an autonomous and self-optimizing multi-phase tubular reactor. In the reactor, a combination of reaction and in situ product removal takes place in a countercurrent flow (Klankermayer, Leitner, Jupke, Rother). For the electrochemical reactor with suspension electrodes (see Figure 22), we strive to elucidate particle cluster formation and particle percolation depending on fluid flow conditions (Wessling).

Lessons learned from the mesoscale will be essential for successful operation on the macroscale. Complex thermodynamic and kinetic models with costly solutions will be replaced by surrogate or hybrid models derived from outcomes of the smaller scales. These models are selected based on the best trade-off between accuracy and simulation time (Mitsos, Jupke). Real-time simulation will be the basis for model predictive control, facilitating continuous optimization of reactor operation based on dynamic inputs [277]. We also focus on implementing of in-line, on-line, and at-line measurement techniques to obtain indicative quantities and enable on-line model parameterization. A dynamically and flexibly operable reactor design will lead to an autonomous and self-optimizing reactor control system to realize an adaptive operation for high yield and selectivity.

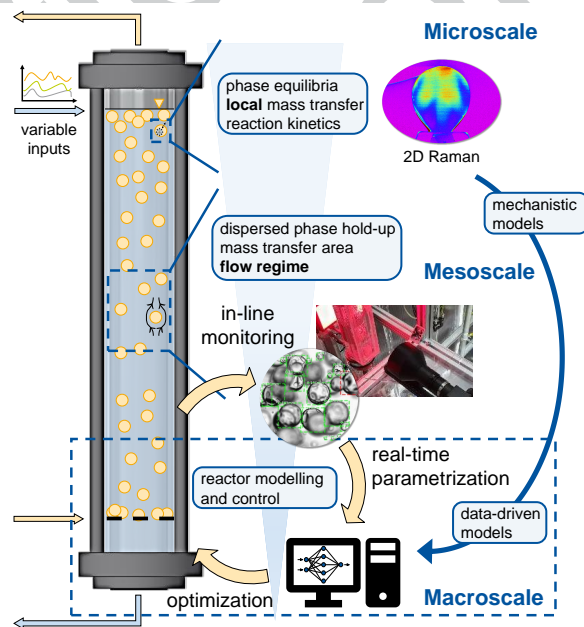


Figure 23: Autonomous and self-optimizing multi-phase tubular reactor.

4.5.3.4 Proposed Staff and Funding of SRA-CSP

Table 4.5.3.1: Proposed Staff in SRA-CSP

Staff category	2026	2027	2028	2029	2030	2031	2032
	Number of persons						
Postdoctoral researchers	3	3	3	3	3	3	3
Doctoral researchers	21	21	21	21	21	21	21

Table 4.5.3.2: Funding Request for SRA-CSP

Funding category	2026	2027	2028	2029	2030	2031	2032
Totals per year in thousand euros							
Staff (Total for 4.5.3)	1607	1639	1671	1705	1739	1774	1809
Direct project costs (excluding staff)	343	463	303	273	258	258	258
Total instrumentation < €150,000	360	355	0	0	0	0	0
Total instrumentation > €150,000	170	0	0	0	0	0	0
DASbox® mini bioreactor system	170						

Instrumentation below 150 000 €

The data-driven development of molecular catalysts requires a high-pressure equipment with adapted analytics (125 k€). To analyze phase equilibria and mixture compositions with little experimental effort, a high-pressure differential scanning calorimetry has to be procured (120 k€). For highly accurate density measurements of liquids over a wide temperatures and pressures range, a high-pressure density meter (50 k€) is required. To gather thermodynamic fluid data through optimal experimental design and minimizing resource use, a 3-phase tailor-made measuring cell (60 k€) shall be procured. A multi-fold parallel pressure reactor is required for testing of solid single atom materials (120 k€). To study electrocatalytic transformations and to perform *in-situ* product analysis during gas fermentation, two NMR benchtop spectrometers are required (140 k€). For evaluating biochemical pathways, an automated microbial genome editing workbench (50 k€) shall be procured. The biosynthesis of monomers from renewable carbon sources require a TOM microbial physiology workbench (50 k€).

Instrumentation above 150 000 €

In addition to the TOM microbial physiology workbench, a DASbox Mini Bioreactor System is required (170 k€).

4.5.4 SRA "Translational Catalytic Processes" (SRA-TCP)

PIs: Leitner, von der Aßen, Blank, Jupke, Klankermayer, Mayrhofer, Mitsos, Palkovits, Pitsch, Rother, Simon, Waldvogel, Wessling, Zobel; ARs: Khetan, Leonhard, Magnus, Wiegand

The translation on new synthetic pathways into robust and yet flexible future processes requires considering essential challenges regarding the complexity and quality variation of feedstocks, the dynamics and fluctuation of renewable energy sources, and the integration of both supplies with the actual catalytic conversion (Figure 34).

Feedstock complexity is particularly challenging for bio-based raw materials and substrates that are often sophisticated mixtures or even composite materials. The fluctuation of renewable energy input adds the challenge of dynamic operation as additional dimension. Therefore, innovative strategies and methods to provide process energy as well as chemical energy are of great interest. Integrating supply and conversion is a major target for CO₂-based processes comprising capture technologies coupled with catalytic transformations. Analysis on a systems

level needs to be linked with the technology progress from the beginning to evaluate and validate the potential benefits of **integration vs connection** of the individual process steps. The translation of synthetic pathways to processes in SRA-TCP thus covers the technology maturity progression from exploratory studies with model substances to validation under realistic boundary conditions.

Strategy and Structure of SRA

The research in SRA-TCP focuses on the impact of **feedstock complexity and its variation** (Sub-SRA TCP-1) as well as dynamic operation resulting from **energy input and fluctuation** (Sub-SRA TCP-2) on the robustness of catalytic processes. In particular, the challenges and opportunities arising from these issues are addressed in the context of **integrated process concepts** (Sub-SRA TCP-3).

The overall transformations under scrutiny are defined either from the progress in SRA-CSP (4.5.3) or from known reaction sequences of major relevance in the context of renewable feedstocks. While specific methodological developments are pushed forward in the three sub-topics individually, cross-fertilization and exchange of know-how is a strategic goal. This is facilitated by selecting certain transformations as common targets in all three sub-topics and as common case studies for the fuel & chemical design process.

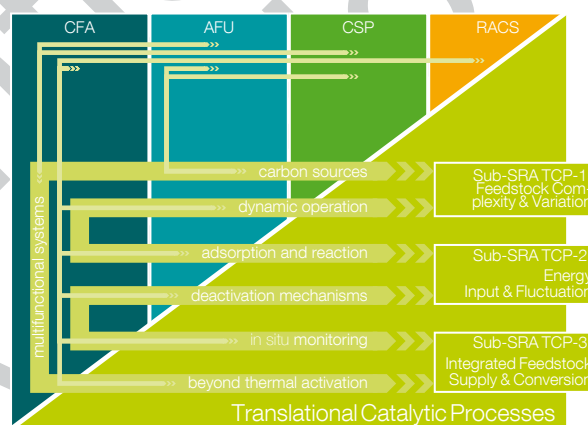


Figure 24: Structure of the SRA-TCP

The leading role of PIs from FSC² in large industrial-academic consortia (Kopernikus, Carbon2Chem, ETOS, Bio4MatPro, CAT Catalytic Center, BioSC, AUFBRUCH) provide detailed insight into the challenges associated with real systems integration. This information provides a unique data basis to design and plan the methodological approaches of the cluster. In selected cases, this valuable network offers access to real industrial feedstocks and energy supply to validate the progress.

4.5.4.1 Feedstock Complexity and Variation

Based on previous experience, FSC² develops a broad methodological portfolio on the chemical deconstruction of the major components in lignocellulose and related polymeric structures. Together with a strong competence in catalytic CO₂ conversion, this forms the basis of the bio-hybrid approach. Understanding and overcoming the challenges of feedstock complexity including impurities, mixtures and variations in composition on different time scales will be the focus of the research in FSC². The incorporation of nitrogen-containing building blocks opens up an additional dimension of complexity for chemo-, bio-, and electro-chemical processes.

Current State of Research and Previous Work

A common strategy to cope with the presence of potential inhibitors is the development of low-cost and low-energy steps for their removal for protecting the bio- or chemo-catalyst from being deactivated. For example, the Toluene diamine (TDA) present in polyurethane hydrolysates from polymer-recycling was identified as major inhibitor with toxic effects on engineered microbes developed in FSC. It was shown that TDAs could be removed from the monomer mixture by reactive extraction allowing successful conversion of the resulting Polyurethanes (PUs) hydrolysate by an engineered microbial consortium to rhamnolipids [112]. A specific microbe could be engineered to produce 3-(3-hydroxyalkanoyloxy)alkanoic acids (HAAs) [113] as platform intermediate for chemo-catalytic or electrocatalytic [207] upgrading to biohybrid fuels or chemicals. In a collaborative effort, the challenge of foaming occurring in such reaction systems at scale was also addressed successfully [115].

For the fractionation of fructose from a glucose-fructose mixture after biomass hydrolysis, selective adsorption was achieved with cross-linked boronic acid polymers. [116]. Selective adsorption proved more generally viable and functional phenylboronate polymers were used for the recovery of biogenic diols from aqueous media [117]. For example, 2,3-butanediol was recovered by this technology from microbial fermentation broth [87]. The application of the polymer adsorption for integrated product removal was demonstrated for production of itaconate by an engineered smut fungus [118–121].

Recently, we could showcase that CO₂-derived substrates such as formate and acetate can be metabolized by smut fungi [65], increasing upon co-feeding significantly the yield of itaconate from glucose. Using CO₂-derived weak organic acids as carbon source for microbes opens novel opportunities for biohybrid production, but requires to decoupling their acidity from the proton gradient of microbes by strain and bioprocess engineering [122, 123]. In the FSC, the synthesis of formate and acetate from CO₂ was studied extensively [63, 124–126]. The products of these reactions might well be suited as substrate for biotechnology even if selectivity is not perfect, because byproducts such as formaldehyde or methanol are readily detoxified by the microbes or ideally used as energy source.

Biotechnological processes such as biogas or bioethanol plants are interesting CO₂ sources in the framework of bio-energy conversion with carbon capture and utilization (BECCU) concepts. Research in the FSC has demonstrated for the first time that CO₂ produced by ethanol fermentation can be hydrogenated *in situ* resulting in combined ethanol and formate synthesis. The breakthrough was possible by finding an operating window where living yeast remained

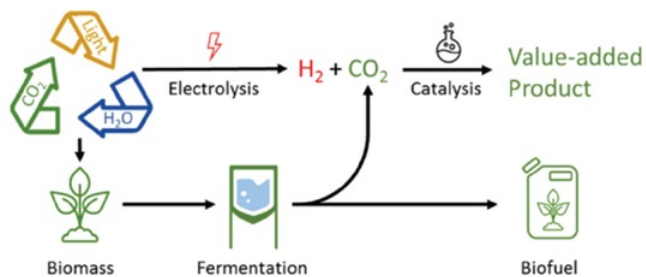


Figure 25: Utilization of renewable resources for biofuel production through fermentation and additional catalytic CO₂-reduction to value-added products. [96]

active under 110 bar of hydrogen pressure and the organometallic catalyst was separated from the fermentation broth in an organic/aqueous biphasic system [96] (Figure 25).

The fuel desing process of FSC has demonstrated the beneficial effects of long-chains alcohols as components in Fischer-Tropsch-based fuels (HyFiT fuels, see section 4.5.1). Based on this fundamental insight, it has been demonstrated as part of the EU project ReDiFuel that the mixture of aliphatic and olefinic products of various chain lengths obtained directly from a Fischer-Tropsch process (“FT crude”) could be hydroformylated and further reduced to the C1 elongated alcohols in a biphasic catalytic system. Observation using a borescope under operando conditions using a specifically designed high pressure reactor was crucial for the understanding of the interplay of molecular mechanisms and the complex phase behavior [127, 128].

Recycled materials are also potential feedstocks facing similar challenges as biomass such as selective degradation and potential catalytic inhibitors. Homogeneous catalysts studied extensively within FSC for biomass and CO₂ conversion proved remarkably robust allowing depolymerisation even for end-user products to provide useful platform chemicals [129]. This provides access to another important source of carbon within the systems boundaries of a de-fossilized value chain [130, 131].

“Green” hydrogen may also show different impurities or by-products depending on its production. While traces of oxygen or water may be contained in H₂ from electrolysis, CO or CO₂ can be present in H₂ obtained from biomass reforming. Interestingly, we found a positive effect of trace amounts of oxygen in CO₂ hydrogenation to methanation doubling the reaction rate of Ni/ZrO₂ at 300°C [209]. Though not fully understood yet, surface hydroxylation facilitating substrate adsorption appears to contribute to this effect. We have also demonstrated that the selectivity for hydrogenation of biomass-derived substrates over certain heterogeneous catalysts depends critically on the use of pure H₂ or H₂/CO₂ mixtures [132]. For example, furfuralacetone is hydrogenated either to the fully saturated alcohol under H₂ or the partially saturated ketone under H₂/CO₂ with high selectivity (Figure 26). The effect is fully reversible and general [133] resulting in adaptive control of product formation depending on the absence or presence of CO₂. *In situ* spectroscopic techniques revealed the reversible formation of surface-bound formate species as molecular reason for the selectivity switch.

In summary, FSC² can build on a large body of experience to study the effects of complex feedstocks at the interface of catalytic disciplines. This allows to define clear objectives for advancing the fundamental knowledge on catalysts and catalytic processes under real-world conditions in the next phase, allowing ultimately for rational process optimization and systems engineering in the future.

Objectives

The objectives comprehend (i) the rational development of robust and flexible (“adaptive”) catalytic systems that can cope with the complexity (composition and variation) of renewable feedstocks. To do so, (ii) the fundamental understanding of the influence of raw material complexity

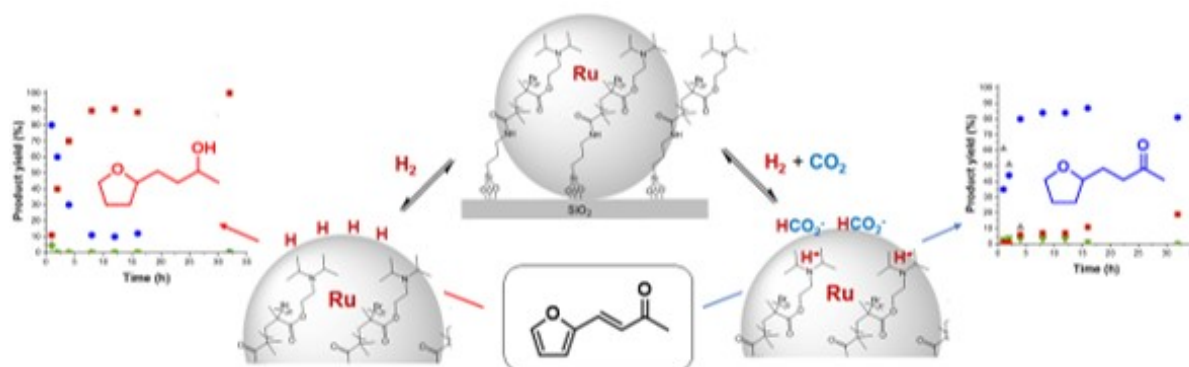


Figure 26: Adaptive catalysis produces either the fully saturated alcohol or the partially saturated ketone from bio-based furfuralactone depending on the use of pure H_2 or H_2 in presence of CO_2 . [132]

on catalyst, transformation, and reaction system will be researched using (iii) experimental and computational techniques to study activation and deactivation processes for such catalytic systems across time and length scales.

Work Program

The development of catalytic systems capable of coping with feedstock complexity requires a detailed understanding of the interaction of the catalytic system not only with the reagents, but also with other components or impurities. The toolbox of methods and techniques to study such phenomena will be expanded and **innovative devices and experimental set-ups** will be designed to provide such insights, for example for liquid and solid-state NMR or X-ray absorption and emission spectroscopy (Wiegand, Zobel). In addition to extensive analytics of pristine and spent catalysts, this includes **operando spectroscopic techniques** that will be **developed and applied in close collaboration between the catalysis teams** on basis of relevant FSC² reaction systems (Blank, Klankermayer, Lauterbach, Leitner, Magnus, Palkovits, Rother). Monitoring the dynamics of the catalytic processes by **online kinetic analysis** for all relevant species coupled with insight into the often **complex phase behavior** of gas/liquid/solid systems will be also integral part of the studies (Jupke, Wessling). **Design of experiments** will be applied for planning and analysis of the experiments. The large body of experimental data will be the basis for analysis by **modeling and simulation** where **algorithm-based methods and ML approaches** will be advanced towards automated screening and self-optimising reaction systems ultimately aiming for achieving predictive potential (Mitsos, Pitsch, Kethan, Leonhard, [278, 279]).

The relevant FSC² reaction systems will focus on catalytic production of bio-hybrid molecules addressing targets relevant for fuel applications, chemical products, and co-production systems. Recent review articles highlight the approaches to be taken on FSC² and outline current trends and future developments [134, 135] [280].

Capitalizing on the very **successful integration** during the last phase of **electrocatalysis and electrosynthesis** in the technology toolbox (see section 4.5.4.2 for details), these developments now provide also the opportunity for research towards translational processes (Mayrhofer, Palkovits, Waldvogel, Wessling). An illustrative example for collaborative efforts with FSC² is the cou-

pling of biocatalytic acetoin formation with electrocatalytic oxidation to butanone overcoming the problem that the electrocatalysis in cultivation broth suffered from parasitic reactions due to dissolved media components [105]. The analytical platform provided by the Mayrhofer group allows specific insights into molecular interactions at the electrode materials particularly relevant for CO₂-based processes [136]. The newly acquired experience of the Waldvogel team with scalable electrosynthetic methods utilizing technical grade feedstocks will be highly beneficial in this context [289] [281–283].

Targeted modifications of the electrode material allows for example to overcome the sensitive to specific impurities as shown e.g. for electro-hydrogenation at nickel foam cathodes that operate even in the presence of sulphur impurities with technically relevant substrates [284]. Reflecting the increasing importance of “green ammonia” at the interface of energy and chemistry, FSC² will **strategically extend** its efforts on catalytic synthesis and processes **towards nitrogen-containing building blocks and products**. FSC² is in a unique position to address the challenges resulting from integrating renewable N-sources into the chemical value chain and to evaluate competing demands (viz. fertilizer, nutrition, hydrogen carrier, fuel) on a systems level. Possible transformations include biotechnological direct N₂ fixation [285] as well as biocatalytic amination reaction [138]. Recent research on homogeneous catalysis also demonstrates the potential to combine biobased feedstocks, syngas, and amines for the construction of nitrogen-based intermediates and products [210]. Promising approaches to activation of ammonia and ammonia-derived building blocks are also offered by electro-catalytic processing options [139, 140] [286, 287].

The challenge of renewable feedstock complexity will be addressed beyond carbon resources as outlined above for the quality of hydrogen or the exploitation of ammonia and nitrogen-based building blocks. Obviously, integration with the energy input is of major importance and the implications of the planned FSC² research on energy integration and fluctuation is explained in the following section.

4.5.4.2 Energy Input and Fluctuation

With electricity from renewable resources **becoming the main energy source for chemical processes**, challenges and opportunities arise to control catalytic transformations on a molecular and process level. In particular, technology options need to be designed **to deal with fluctuation** of the primary energy source **in a flexible and even adaptive manner** beyond simply replacing thermal with electrical heating. The cluster research in this area will focus on **electrocatalysis, mechanochemistry, and magneto-induced catalysis**.

Current State of Research and Previous Work

Electrochemical approaches to drive CO₂ and biomass conversion have been integrated in the FSC consortium strategically in the previous phase and extended to more complex synthetic processes with the recent appointment of Prof. Siegfried Waldvogel as Director of the new Department of Electrosynthesis at MPI CEC. Based on his pioneering work introducing

electrosynthetic conversions as widely applicable tool in organic chemistry, he has recently provided examples how its combination with intermittent electricity from renewable this can be a very green option for chemical transformations [284]. For oxidative aromatic C-C coupling, a class of important technical reactions, it was shown that robust conversions allow alteration of current density by several orders of magnitude without loss in selectivity [288] (Figure 27). The applicability to syntheses utilizing nitrogen-based building blocks was also demonstrated [289].

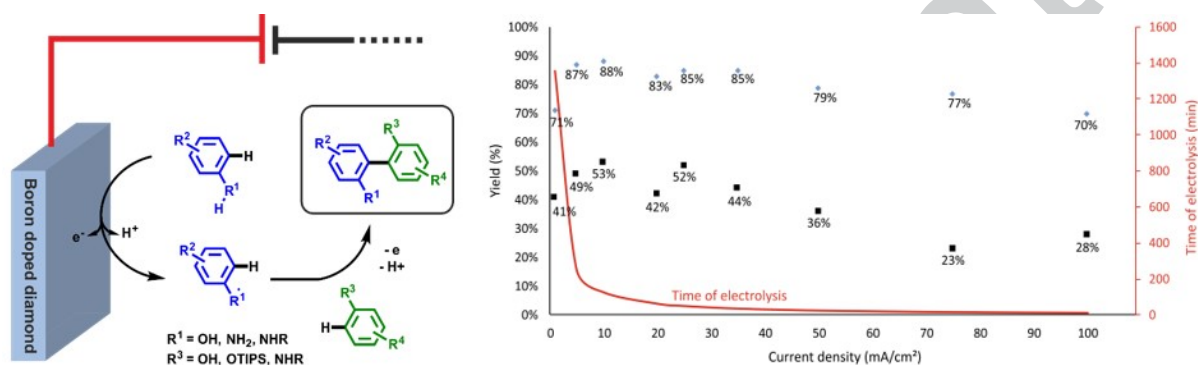


Figure 27: Highly robust electrochemical C-C coupling allows to reduce the reaction time (red line) from over 20 h to less than 2 h at high current densities.

A key factor for the rapid and potentially adaptive transfer of the electric power into chemical reactivity are interfacial processes between the electrode material and the reactive intermediates. 3D structured electrodes have been studied in detail and novel methods for their fabrication [211] have been developed. While the generation of hydrogen as such is not in the focus of FSC², the direct relay between proton reduction and chemical reactions utilizing the anodic oxidation potential offers a very attractive opportunity to couple dynamics of the supply with catalytic steps [141, 142]. Another possibility is the direct coupling of the H₂ production with catalytic hydrogenation, whereby the interfacial phenomena have to be controlled in addition between the aqueous electrolyte and the hydrophobic substrates [143].

Mechanochemical activation through ball milling has been demonstrated as promising approach to ensure intimate contact between complex solid feedstocks and solvents or reagents facilitating their breakdown to intermediates and building blocks. Vice versa, reactions of solid reagents or catalysts with gaseous feedstocks such as CO₂ can be conducted very effectively under ball milling conditions [73]. Most recently, the potential to activate nitrogen-containing intermediates and building blocks has been demonstrated paving the way towards potential ammonia conversion strategies [212, 213]. The potential of solid state NMR to obtain fundamental insights into mechanochemical processes has been demonstrated and critically discussed [290] (Figure 28). Notably, a Faraday Discussion meeting has been co-organised by PIs from FSC to foster the community building in this innovative area [291].

Magnetic induction provides an effective tool for very localised heating reacting instantly to dynamic changes in the power supply. Pioneering research within FSC has demonstrated the possibility to decorate traditional and even commercially available heterogeneous catalysts with magnetically responsive nanoparticles [214]. The reverse catalyst design to use the iron carbide nanoparticles (ICNPs) as support for active metal nanoparticles has also been established [215].

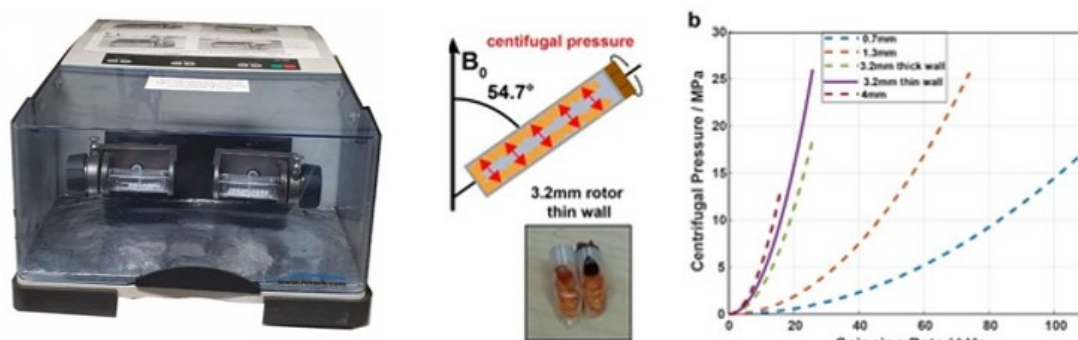


Figure 28: Solid-state NMR to study the activation mechanisms in mechanochemical processes.

Due to very high specific absorption rates (SARs) under alternating magnetic fields, ICNPs were shown to allow catalytic hydrogenation and hydrogenolysis under significantly lower bulk temperatures due to local hot spot formation. Most significantly, the immediate response of the catalyst to applying the electric current to generate the magnetic field was demonstrated to enable real-time on/off switching of the catalytic activity (Figure 29).

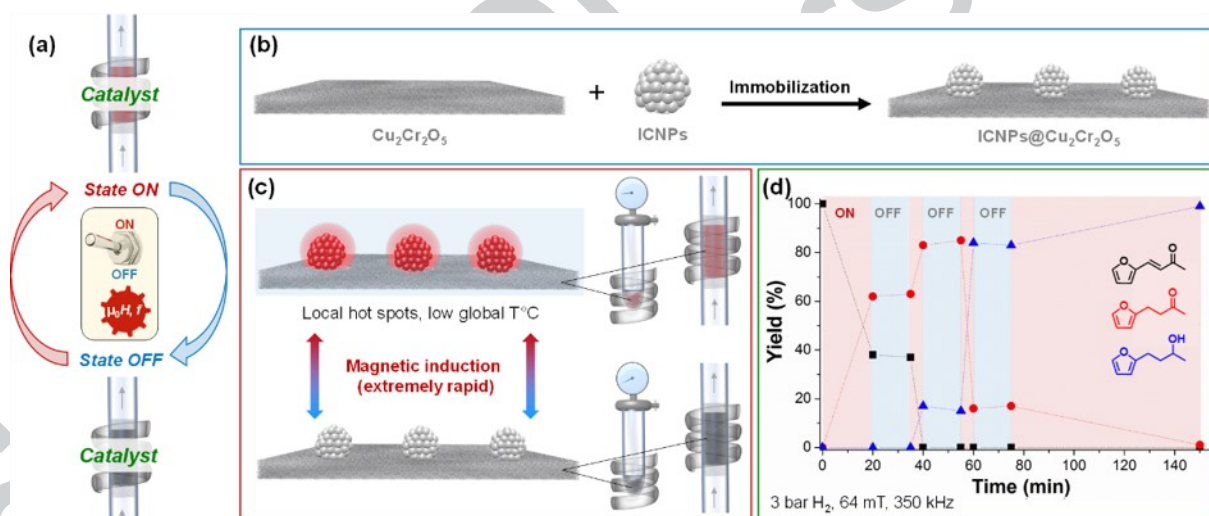


Figure 29: Magnetic induction heating as trigger for real-time activation of catalytic performance in response to electricity supply.

Objectives

The research in Sub-SRA TCP-2 will provide the basis for the design and demonstration of **adaptive catalytic systems** in response to fluctuations in primary energy supply. Alternative methods for **rapid energy input** in catalytic systems will be developed **utilizing electro-, mechano-, and magneto activation**. The potential for **reversible adjustment of different reactive states** of the catalysts will be evaluated. The **fundamental understanding of activation and de-activation processes** within the catalytic system on molecular level and across material interfaces will provide essential design criteria for **robustness** of the systems.

Work Program

For electrochemical and electro-catalytic processes, a number of different approaches can be envisaged and will be addressed in individual projects (Waldvogel, Wessling, Palkovits, Mayrhofer, Lauterbach, Simon). We highlight here the use of flow electrodes, which consist of conductive particles suspended in the electrolyte, as they are promising for increasing the active electrode area without increasing the reactor footprint. The charge transport mechanisms in flow electrodes remain unclear because the occurring phenomena are fast and highly complex. Based on previous work by the Wessling group [110], the greatest effect on the electrical conductivity can be associated with the formation of particle bridges resulting from the electrical percolation networks between the electrodes (Figure 30). Such insights will be used to translate the concept into electrocatalytic processes and electrosynthesis more broadly within the team.

While the number of catalytic processes demonstrated under mechanochemical conditions increases rapidly, the detailed mechanisms of energy input and interfacial phenomena remain poorly understood and will be studied in particular by NMR and other spectroscopic techniques (Bolm, Wiegand, Zobel). The potential for reactivity and in particular selectivity control through variation of the agitation power has so far not been explored systematically and could open a new area of applications.

With the recently established reactor systems to conduct magneto-induced catalytic reactions in continuous flow [214] under online and inline analysis (Figure 31), the potential of this innovative method will be broadly explored (Leitner, Jupke, Khetan). In particular, technical solutions to conduct such reactions under elevated pressure will be highly beneficial for the synthesis of bio-hybrid fuels and chemicals involving hydrogen, carbon monoxide, and carbon dioxide. A major goal for the fundamental understanding of the control factors is the exact measurement of the local temperature and its dissipation into the catalytic active material and into the reaction medium. Combinations of processes requiring very different temperature regimes might become feasible in an unprecedented manner (for example see Sub-SRA TCP-3, integrated CO₂ capture and conversion).

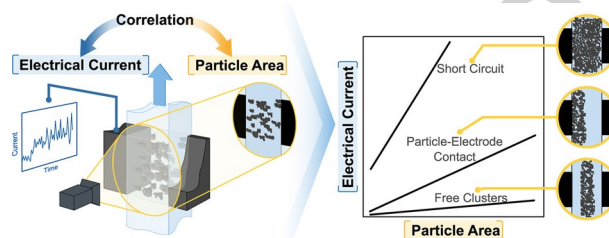


Figure 30: Flow electrodes consisting of conductive particles suspended in the electrolyte increase the active electrode area without increasing the reactor footprint.

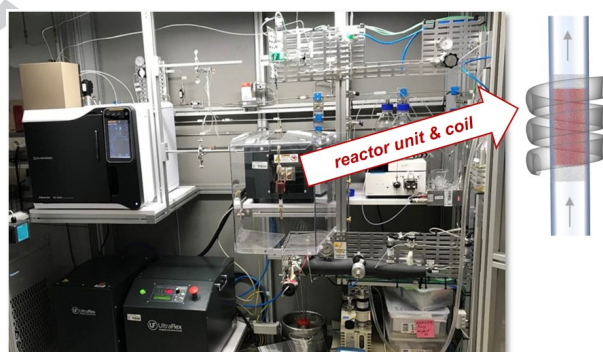


Figure 31: Continuous-flow reactor for magneto-induced catalysis.

4.5.4.3 Integrated Feedstock Supply and Conversion

Based on a fundamental understanding of the influence of raw material complexity and energy supply on catalytic processes, it becomes possible to tackle an integrated supply and conversion of real feedstocks in a potentially variable or even adaptive manner. For feedstocks such as CO₂, an integrated supply, separation, and conversion can be envisaged valorising bio-, chemo-, or electrocatalytic transformations.

Current State of Research and Previous Work

Within the diverse feedstock base, CO₂ poses specific challenges. It can be provided in pure form by direct air capture (DAC) associated with high energy demands. Alternatively, CO₂ is available in form of carbonate or amine solutions from scrubbing processes or even as (highly) diluted and multi-compound feed stream directly from air or other chemical processes. Accordingly, suitable approaches for integrated feedstock uptake and conversion require both a high degree of flexibility and robustness. Environmental merit order curves were developed to rank CO₂ sources according to their environmental impact over the available CO₂ supply to

identify favorable locations for CO₂ utilization with lowest environmental impacts, so-called CO₂ oases (von der Aßen). [145, 146] To enhance efficiency of carbon capture, advance in tailored adsorbents, adsorbents, as well as process design were targeted. Tailored adsorbents bear the potential to significantly reduce the energy demand of DAC. Previous studies highlight the potential of N-containing carbon materials enabling high CO₂ capacity and selectivity. Material morphology and surface functionality were identified as major design criteria for covalent triazine frameworks (CTF). With CO₂ uptakes of up to 5.97 and 4.22 mmol g⁻¹ at 273 and 298 K, competitive materials could be provided ranking among the best reported in literature CTFs (Figure 32) [144]. Also, polyacrylonitrile-based carbon nanofibers (CNFs), prepared at different carbonization temperatures, enabled efficient CO₂ sorption with measured CO₂/N₂ selectivity of up to 194 [147]. In contrast to packed beds, hollow fiber, or tubular, adsorption devices facilitate controlled flow conditions, low pressure drop, and facile scale-up via numbering up. CNT-based microtubes were impregnated with polyethylenimine and employed for temperature swing adsorption of CO₂. A module with multiple tubes in parallel enabled scale-up, and load-flexible operation. Overcoming the need for thermal energy for desorption, the tubular adsorbents were adapted allowing direct Joule heating of silicon carbide or zeolite enforced fibers [148].

ICCC enables overcoming sequential CO₂ capture, storage and release of CO₂ followed by its conversion. In FSC, direct hydrogenation of CO₂ contained in an amine scrubbing solution to formate was demonstrated. The type of amine had a distinct effect on catalyst activity stressing the importance for integrated development [149]. Also for high temperature co-electrolysis of

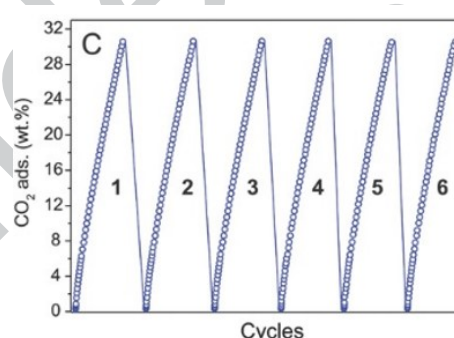


Figure 32: CO₂ sorption cycles at T = 273 K on a high temperature treated pyridine-based CTF confirming high stability. [144]

4 Research Program

CO₂ and water to CO and H₂ followed by CO₂ hydrogenation, direct integration was possible [150]. The water content of the feed from co-electrolysis proved crucial for catalyst activity and stability. While a commercial Ni/Al₂O₃ catalyst showed fast deactivation for water contents exceeding 10 %, tailored NiFe/(Mg,Al)O_x could even operate at 30 % water content and was readily regenerated by calcination.

In the thermo-catalytic hydrogenation of CO₂ to produce carboxylic acids, activity and selectivity could be significantly enhanced by supplementing the primary liquid decane reaction by a second methanol product conservation phase allowing continuous extraction by an acid-amine complex [151]. Another two-phase system [96] was applied to utilize the co-produced CO₂ of a bioethanol fermentation as a feedstock for a homogeneously catalyzed hydrogenation to formic acid. A novel tool was developed facilitating pH-control without the need for acids and bases, significantly reducing the co-produced saline waste. The tool electrochemically produces H⁺- and OH⁻ ions for pH control. It was applied to develop *in situ* purification processes particularly for microbially produced carboxylic acids [152].

Beyond CO₂, also the selective separation of biomass-based intermediates such as sugars, carboxylic acids, amino acids and diols [153] from complex mixtures has been demonstrated enabling novel integrated processing strategies. In a case study on itaconic acid, selective separation from crude fermentation broth was possible with novel adsorbent systems. However, electrocatalytic studies have highlighted the possibility to directly convert biotechnologically derived platform chemicals such as itaconic acid or HAAs without any prior separation [105, 154].

Objectives

The objectives comprehend (i) identifying the potential of dynamically operated processes that can cope with variable feedstocks and energy supplies. This requires (ii) a fundamental understanding of trade-offs in valorising real-world feedstocks by intensified process concepts compared to sequential separation and conversion. As a prime example, (iii) enabling tools and design criteria for an integrated separation and catalytic transformation of CO₂ feed streams will be researched.

Work Program

The purification and compression of CO₂ prior to a reduction reaction are both energy-intensive steps. The ICCC promises more energy-efficient processes. In an ICCC process, the provision of a highly concentrated CO₂ gas phase is omitted by directly converting the sorbent-bound CO₂, instead of releasing it into a gas phase. The degree of integration of both process steps can vary strongly. Thus, we aim to address ICCC on three layers: the catalytic layer (Leitner, Palkovits, Wessling), the device/process layer (Wessling, Jupke), and the system layer (von der Aßen). In thermo-catalysis, temperature management of integrated reaction concepts presents a major challenge as adsorption and catalytic transformation require different optimum operating temperatures. Magnetic induction heating/cooling of magnetic nanoparticles will be

utilized to provide rapid adsorption/reaction swings to a multifunctional catalytic system capable of capturing (low T) and converting (high T) CO₂ thus may allow bringing CO₂ capture and conversion together (Leitner). On the molecular level, orthogonal material design will enable integrating tailored sorption sites and catalytically active centers for valorizing sorption-enhanced catalysis (Palkovits). Conceptually, sorption sites close to the active centers cause locally enhanced substrate concentrations directly translating into superior reaction rates far beyond the limitations of the bulk feed concentration.

Absorption systems for CO₂ are often of aqueous nature fostering the dissociation to H₂CO₃, HCO₃⁻ and CO₃²⁻. For selective conversion of absorbed CO₂ meticulous control of the local pH must be achieved. Two conversion pathways will be investigated leveraging precise control of catalyst boundary layer species concentrations in thermo-catalytic bicarbonate conversion and bicarbonate electrolysis. In the first pathway, alkaline scrubbing is used to separate CO₂ from flue gas or air (DAC) leading to the formation of bicarbonate/carbonate. The recently developed heterogeneously catalyzed formic acid production from bicarbonate/carbonate in aqueous solution serves as compatible conversion system. Integrating capture and conversion is enabled by a closed-loop operation requiring electrochemical pH control to avoid the accumulation of co-ions. Whereas the base regenerates the absorption capacity of the alkaline scrubbing unit, the acid protonates the carboxylic acid produced in the CO₂ conversion step. Several fundamental challenges need to be addressed. First, the catalytic system of the mono- or dicarboxylic acid producing reactor must be adapted to a bicarbonate/carbonate feedstock and improved with respect to efficiency and productivity (Palkovits, Blank, Jupke). Opposed to the thermo-catalytic approach suggested in literature, a bio-catalytic conversion will also be considered. Second, the complex interactions between the bicarbonate/carbonate provision, the hydrogenation, and the hydrogen supply must be aligned to operate the conversion unit. For that purpose, equilibria and kinetic rates of the hydrogen absorption, the dehydration reaction of bicarbonate/carbonate and the hydrogenation reaction in the heterogeneous catalyst layer are experimentally explored. Based on the acquired data, a locally resolved reactor model is set up to facilitate the design of the conversion unit. Finally, an electrolyte composition must be identified that fits the requirements of all unit operations: CO₂ capture step, the electrochemical pH swing cell and the conversion unit. In the second pathway, direct electrochemical bicarbonate electrolysis will be explored, which can be integrated with gas scrubbing (Wessling). For high Faraday efficiencies and carbon utilization, pH and concentration control at the catalytic interface is of pivotal importance, as it defines the equilibrium of carbonate species and thus, the reactive substrate. Classically, bipolar membranes are aligned adjacent to the cathode to supply protons and thus impose the desired pH gradient to push bicarbonate to dissolved CO₂, which reacts at the electrode interface. With precisely designed porous 3D electrodes via additive manufacturing we aim to control mass transfer and pH gradients inside the porous electrodes and thus ensure sufficient reactant availability while preventing oversaturation of the electrolyte and subsequent CO₂ bubble formation. To locally control species concentration, we will investigate pulsed electrolysis for boundary layer relaxation. Pulse duration, symmetry and amplitude decisively affect local concentrations and thus, the conversion

path. By combining continuum modeling simulations with experimental investigations of the electrode/electrolyte interface in micro- and macrofluidic devices, we gain detailed understanding of the levers towards increased selectivity. Multiphase modeling (Pitsch) will accompany dedicated experiments to elucidate bubble nucleation, detachment and removal in complex electrolytes and electrode structures. Special emphasis is put on the requirements of the integrated CO₂ absorption and conversion unit, as it has been shown that the CO₂ conversion unit does not perform well if designed to fully comply with the absorption inlet and outlet stream. Additionally, the influence of additives and impurities remains largely elusive and will be assessed. At last, device level integration is pursued by developing next generation bipolar membranes. Bipolar membranes have recently shown great potential to reach satisfactory current densities. However, stability in highly concentrated electrolyte solutions must be achieved by tailoring the individual ion exchange layers and bipolar junction.

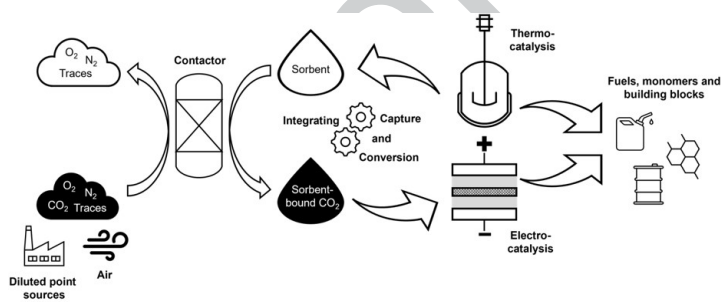


Figure 33: Integrated capture and thermo-catalytic or electro-catalytic conversion of sorbent-bound CO₂ to fuels, monomers and building blocks.

On the system level, the methodological concepts are mirrored in dynamic modeling of material behavior and LCA for designing sustainable integrated carbon capture and conversion processes in volatile energy systems (van der Aßen).

4.5.4.4 Proposed Staff and Funding of SRA-TCP

Table 4.5.4.1: Proposed Staff in SRA-TCP

Staff category	2026	2027	2028	2029	2030	2031	2032
	Number of persons						
Postdoctoral researchers	3	3	3	3	3	3	3
Doctoral researchers	14	14	14	14	14	14	14

Table 4.5.4.2: Funding Request for SRA-TCP

Funding category	2026	2027	2028	2029	2030	2031	2032
	Totals per year in thousand euros						
Staff (Total for 4.5.4)	1233	1258	1283	1308	1335	1361	1388
Direct project costs (excluding staff)	248	328	228	228	228	228	228
Total instrumentation < €150,000	375	130	60	0	0	0	0
Total instrumentation > €150,000	170	160	0	0	0	0	0
DASbox® mini bioreactor system	170						
Online analytics (e.g. NMR, GC)		160					

Instrumentation below 150 000 €

For the investigation of ordering phenomena and molecular interactions in immobilized catalysts by solid-state NMR spectroscopy, a HXY triple-resonance solid-state NMR probe (500 MHz, also capable for low-gamma nuclei) has to be procured (100 k€). For the detailed analysis of the sample composition as basis for calculation of the neutron scattering length of complex catalytic systems, CHNO analysis is required (120 k€). A Bruker IR 70V spectrometer is required for the operando spectroscopy of molecular catalysts (130 k€). To enable the identification of phenomena sensitive to fluctuations, facilitating autonomous, and resilient operation, a multi-phase reactor (60 k€) is required. An experimental setup for the operation at elevated current densities and potentials is required (85 k€) to the sustainable formaldehyde production using Faraday efficiencies of up to 90 %. For the MW-enabled ICCC, a MW-cavity for X-Ray spectroscopy and diffraction is required (70 k€).

Instrumentation above 150 000 €

For the investigation of aceton-butanol-ethanol fermentation concepts, a Dasbox is required (170 k€). To monitor the process states of the multi-phase reaction system online to examine different continuous operating points and align the complex interactions between the bicarbonate/carbonate provision, the hydrogenation reaction system, and the hydrogen supply, an Online analytics suited for high temperature reaction systems shall be procured (160 k€).

4.5.5 SRA "Resilient & Adaptive Conversion Systems" (SRA-RACS)

PIs: [von der Aßen](#), [Walther](#), Arning, Leicht-Scholten, Mitsos, Greiff; ARs: Backhaus, Venghaus, Ziefle

We develop an integrated approach for the design & operation of fuel & chemical conversion systems to be both resilient to withstand and quickly recover from disruptions, and to be adaptive to adjust to variability in short-term supply and demand and long-term transformation processes. The approach will encompass all dimensions of sustainability, economic, social and environmental. Also, it will be integrated over all levels, from the product, to devices & processes, to the broader supply chain and system level. The approach consists of [Fuel and Chemical Design](#), [System Integration](#) and [Sustainability Assessment](#).

Strategy and Structure of SRA

The transition toward climate neutrality drives the rapid convergence of chemical, fuel, and energy systems. This shift necessitates a holistic perspective on the entire fuel and chemical conversion system, fostering adaptability to feedstock variability and asking for an integrated design of fuels & chemicals, and product & process. Therefore, we develop the integrated [Fuel & Chemical Design Process \(FCDP\)](#), incorporating objectives of resilience, adaptivity and sustainability to process design and integrated process/product design. The feasibility and sustainability of the developed process paths, chemicals, and fuels must then be evaluated within

a broader system context, considering also alternative and complementary process paths, energy carriers, and products as well as limited availability of energy sources and feedstocks at global scale. These global conversion systems must be designed to be resilient, i.e., capable of overcoming (geo-)political, technical, economic, environmental, natural, and social risks.

In **System Integration**, we therefore expand the scope towards such a global system's perspective to design resilient and adaptive fuel and chemical conversion system merging system analysis with stakeholder-specific decision-models, ex-ante systemic risks assessment, prospective policy design, and dynamic transformation processes. Moreover, global fuel and chemical conversion systems must also be designed to be sustainable, i.e., adhere to planetary boundaries while still meeting societal needs. Thus, we will extend the life-cycle assessment

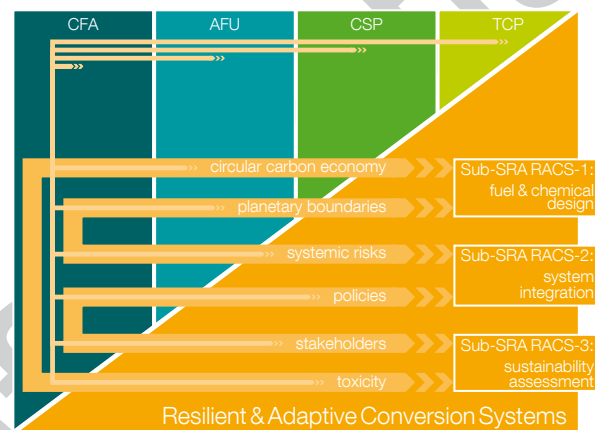


Figure 34: Structure of the SRA-RACS

methodology to a **Sustainability Assessment** to capture the sustainability impacts of fuels and chemical conversion systems over all scales. While the LCA methodology and environmental impacts will remain a focus, socio-economic impacts from the System Integration will also be included. Ultimately, the Sustainability Assessment indicators will be used as environmental objective in the **FCDP**. The goals of SRA-RACS are resilience and adaptivity across scales. We will unify the definitions of resilience and adaptivity, as the SRA involves multiple disciplines that currently do not have a uniform understanding of these terms. We will formalize these mathematically so that we can include them in the design optimization of the FCDP.

The results of SRA-RACS are fed back to the other SRAs consistently to enable an iterative research process within FSC² based on an ex-ante evaluation of developed process paths and fuels.

4.5.5.1 Fuel & Chemical Design

We extend our successful fuel design methodology to account for simultaneous fuel & chemical design and the design & operation of resilient and adaptive sustainable production processes. In the integrated product and process design, we account also for propulsion and thus the entire conversion chain. We develop and apply cutting edge methods, including machine learning. Through the Fuel & Chemical Design Forum (FCDF) (see Section 5.4.3), the research is tightly integrated within the whole FSC².

Current State of Research and Previous Work

Several groups have developed methodologies for process design for sustainable chemicals and fuels, e. g., [292, 293]. Molecular design as well as combined molecular and process design is also a very active research field, e. g., [294], including the use of machine learning [295].

The involved PIs have great experience in the design of chemical and energy systems. In particular, we have bridged process & product design, as well as production & propulsion, e. g., [5, 155]. Moreover, we have been very active at the intersection of energy and chemical processes, e. g., [216]. Electrochemical systems play an increased role within FSC, both for the production and propulsion. These will be considered in the fuel & chemical design, and our experience with modeling of electrochemical conversion systems is thus very important, e. g., [217].

Incorporating adaptivity and resilience onto chemical & fuel design will result in numerically very challenging optimization problems [296, 297]. We have lots of experience with similar optimization problems. For instance we have developed dedicated mathematical formulations that consider variability and uncertainty for the planning and scheduling of chemical and energy processes and overcome the limitations of standard formulations [218]. The resulting optimization problems fall in the class of robust nonlinear programs for which we have best-of-a-kind algorithms released as open-source optimization tools⁸. To ensure numerical tractability we will also rely on surrogate data-driven models of parts of the process and we have been at the forefront of combining such surrogates with rigorous optimization [219].

Objectives

The Fuel & Chemical Design aims to overcome the limits of current production processes which exhibit insufficient flexibility to cope with volatility of renewable energy and feedstocks and in economic boundary conditions. Moreover, we have the methodological goal to extend the fuel design to new boundary conditions, e. g., drop-in fuels for ship combustion engines and fuel cell-based propulsion. Further, we have the application-oriented objective to identify critical green chemicals to enhance the resilience and adaptivity of fuel, energy, and chemical systems despite extreme uncertainties. Finally, we plan to incorporate novel intensified and electrochemical unit operations in process operation.

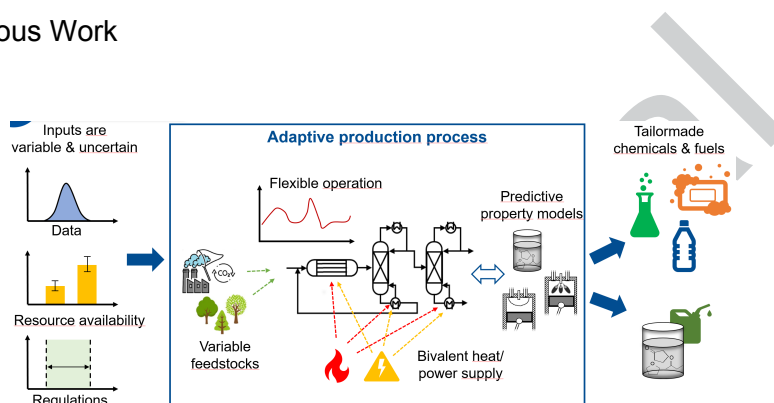


Figure 35: Fuel & chemical design for resilience and adaptivity

⁸<https://git.rwth-aachen.de/avt-svt/public/libdips>

Work Program

The fuel and chemical design is at the core of FSC². We will continue the development and use of methods for the integrated fuel/chemical and process design. In particular, we seek to find optimum tradeoffs between best fuels, most profitable chemicals and best production processes (Mitsos, von der Assen). We utilize model-based optimization-assisted design. The models consider the whole conversion from production to propulsion. Regarding propulsion, we distinguish between (i) combustion engines vs. (ii) fuel cells. In addition to the conversion processes we also account for the supply chains, both for the required feedstock/energy sources and for the distribution of chemicals and fuels (also see System integration in Section 4.5.5.2) using coupled supply chain, process, and combustion models (Walther, von der Assen, Mitsos).

For the combustion engines we focus on fleet-compatible options to account for the fact that sustainable fuels are needed now and at least for the next decades (Pitsch, Mitsos). In particular, we emphasize optimization-based identification of drop-in fuel including oxygenated blending components and production process including integrated carbon capture and conversion (von der Assen, Mitsos). Mathematically, these problems result in large-scale mixed-integer programs, including nonlinearities arising from accurate description of production and propulsion.

In contrast to previous works, we will also account for novel propulsion systems (developed in SRA-CFA & SRA-AFU), such as direct liquid fuel cells (Mitsos). To integrate the performance of such novel propulsion systems in integrated process & product design, predictive models of the performance of the fuel cells are required, accounting for the influence of degree of freedom. We will base these models on our prior work as well as literature contributions. Mathematically, the optimization formulation are similar to the case of combustion engines.

The fuel and chemical design accounts for degrees of freedom in both molecular and process level. To enable this, we employ predictive fuel blend property models for material compatibility, toxicity, and emission formation (Backhaus, Pitsch, Mitsos). These will be based on high-order graph neural networks (GNN), enhanced by imposing physical relations in the training of the networks. In other words, we extend the very successful concept of physics-informed neural networks from partial-differential equations to prediction of relevant physical properties. Moreover, we will couple with a-priori calculations, including reactive Molecular Dynamics in our ChemTraYzer (CTY) tool (Leonhard). Mathematically, the inclusion of the GNNs results in a substantial increase of the size of the optimization formulation; utilizing our ideas of reduced-space formulations, we expect the problems to remain tractable (Mitsos).

A particular focus in the coming years will be to incorporate the objectives of flexibility, resilience, and adaptivity into the process design. The first step will be to unify the definitions of these concept among the disciplines involved in FSC (Walter, Mitsos). Accounting for these important properties, implies the need to combine two-stage stochastic and robust approaches to model uncertainty. While these two ways of modeling uncertainty are typically used separately, the reality of fuel and chemical design requires their combination. Mathematically, these problems amount to hierarchical optimization problems, which are notoriously challenging. In the case of fuel and chemical design, the problems however exhibit a decomposable structure;

by extending our existing methods and tools to account for this structure, we expect to obtain tractable formulations. This will allow us to optimize a portfolio of green chemicals for resilient and adaptable supply system (von der Assen).

Overall, the desired tasks result in very challenging mathematical formulations. We plan to utilize data-driven surrogate models, based on machine learning concepts, to overcome computational expense. (Mitsos) In particular we plan to extend our work on hybrid mechanistic/data-driven and apply it to the fuel and chemical design.

4.5.5.2 System Integration

The aim is to design resilient, adaptive, and sustainable conversion systems for fuels and chemicals using an integrated approach based on system analysis, risk assessment, stakeholder-specific decision models, and policy design. We analyse the feasibility and system integration of the fuels and process paths developed by the other SRAs, and extend the system boundary towards competitive and synergistic process paths, technologies and chemical energy carriers. We apply qualitative and quantitative social and risk sciences methods, data mining, machine learning, as well as agent-based simulation and optimization for system analysis and design.

Current State of Research and Previous Work

In Competence Area 3 (CA3), an interdisciplinary team of researchers from biology, engineering, economy, and social sciences followed a [system-wide design perspective](#) to guide and evaluate novel transformation pathways for the transformation towards flexible value chains for bio-hybrid fuels, integrating techno-economic, sustainability, and social aspects, as well as policy implications.

The development of such integrated approaches requires [inter-sectoral, high-resolution data and scenarios](#) [298]. Analyzing supply chain stages and their interlinkages showed how short- and long-term availability of feedstocks determines technology choice and structure of supply chains [156–158]. (Meta-)analyses provided predicted future demand of fuels for different scenarios [159]. Prospective fuel candidates were determined regarding market diffusion barriers and sustainability factors with a possibility-based multi-criteria approach [160, 161]. Extending studies that analysed [barriers for diffusion of individual fuels](#), e. g. [299, 300], a combined micro- and macro-level approach over different fuel alternatives confirmed economic and technical supply chain challenges, lacking public perception, insufficient regulation and policies, missing stakeholder coordination, lacking feedstock availability,

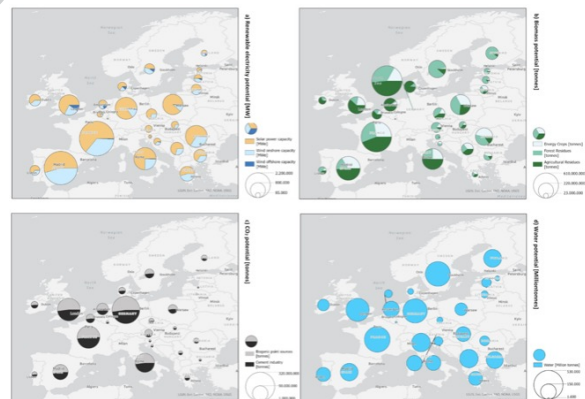


Figure 36: Potential of resources in EU countries a)Renewable electricity potential b)Biomass potential c)CO₂ potential d)Water potential [156]

confirmed economic and technical supply chain challenges, lacking public perception, insufficient regulation and policies, missing stakeholder coordination, lacking feedstock availability,

and environmental challenges as main barriers [160].

To account for the central role of **public perception** [301], the multi-faceted perspective of risks and benefits of fuel products, production processes and infrastructural changes was analysed based on a multi-stage iterative empirical methodology [162]. Research revealed acceptance and risk perception of fuels as a complex construct, segmented into distinct domains such as health, environment, and technical risks, and influenced by cognitive and affective components and individual factors [163]. A positive perception of alternative fuels requires social adaptability and affordability as well as environmental benefits and toxicity concerns of fuels along with infrastructural developments and political communication [164]. Communication of benefits can strongly improve perception of sustainable technologies, but there is the danger of misconceptions, especially for innovative technologies with little prior knowledge of the lay public.

To account for the high impact of **policies** [302, 303], a comprehensive analysis of European, national, and regional policies across multiple scales and sectors showed that synthetic (bio-hybrid) fuels are covered primarily in selected energy and specific hydrogen-related policies, but not included in other relevant policy fields like biomass utilization, bio-economy, water, or environmental policies [161]. Also, the techno-economic and social perspectives are only insufficiently considered compared to the environmental perspective. To allow for better informed decisions, a new distance-to-ideal-solution approach was developed to better regard for expert opinions (policy makers, investors, R&D) on environmental, social, and economic aspects of renewable energy systems [165].

Models for the **design of fuel conversion systems** have to account for long-term transformation, feedstock variability, import scenarios, and high integration of the fuel and energy sector [304]. Often, prescriptive optimization is used for the design of either energy systems, e.g. [305, 306], or fuel supply chains, e.g. [307, 308], with few integrated approaches [309, 310] mostly either for biobased or e-fuels [311, 312]. We enabled sector-integration by model extension. An energy system optimization model was extended to investigate interdependencies between synthetic fuel production and required investments and dispatch in infrastructures for electricity, hydrogen, methane, and liquid fuels [158, 167–169]. Myopic solution approaches proved appropriate, reducing the computation time drastically while still providing adequate objective values [158]. A value chain model was extended integrating investment decisions for renewable energy provision, herein capturing long-term planning horizons for the transformation towards climate-neutrality as well as short-term variability of feedstocks by cyclic time de-

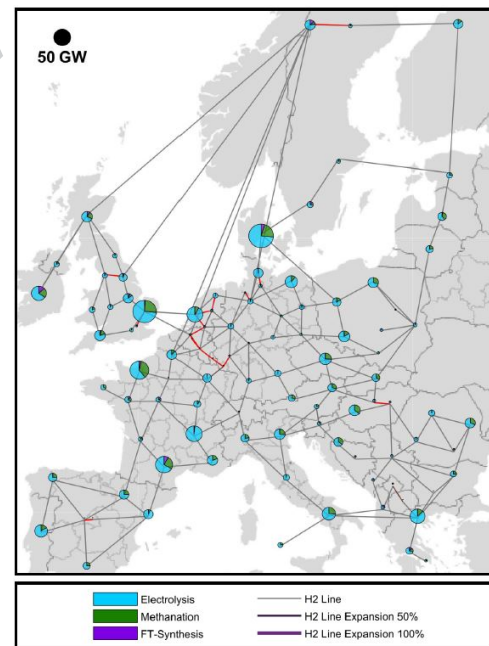


Figure 37: Potential Distribution of Power-2-X Plants in 2050 [166]

composition [157]. A case study with detailed spatial, temporal, and technical resolution for Europe 2030–2050 showed that synthetic fuels are likely to be imported to Europe while synthetic hydrogen could be produced domestically [166]. Model extensions explored the trade-offs between cost, land-use, and water-use [156], the consideration of policy requirements [220], and the innovative integration of social acceptance when designing bio-hybrid fuel supply chains via multi-objective optimization [170, 171]. Potential global energy trade scenarios were analyzed balancing inequality, measured by the Gini-coefficient as per capita economic value added by energy production, with cost [172].

Objectives

An integrated approach is developed for the design and operation of resilient and adaptive conversion systems for energy carriers and chemicals merging system analysis and systemic risk assessment with stakeholder and policy analysis to achieve resilient system design. The approach **extends the system boundary** to account for multi-sectorial effects between the energy, mobility, and chemistry sector over all stages from device over process paths to supply chains, and to regard for the global perspective of value chains. A **systemic risk assessment framework** allows to quantify and evaluate the impact and interrelations of endogenous and exogenous transformative and operational risks as well as acceptance requirements and risk perceptions. A predictive **agent-based approach** enables the explicit recognition of stakeholders' perspectives and their influence on the overall conversion system and vice versa. A **prescriptive policy design** allows for a proactive and iterative configuration of legal frameworks and policies, enhancing the systems' adaptability to emerging risks and changes.

By integrating these tasks, we will be able to **design resilient and adaptive conversion systems** based on long-term system transformation and cross-sectorial system design, while accounting for trade-offs and risks regarding overall system and stakeholders' perspectives and optimal supporting policies. This integrated framework will derive recommendations for the design of resilient and adaptive conversion systems, allow for a better understanding of fuel and chemical conversion systems, stakeholders perceptions and objectives, systemic transformation, and systemic risks.

Work Program

A **multi-sectoral global conversion system model** is developed that represents an integrated perspective on the transformation processes of the energy, mobility, and chemistry sectors. This requires strong cooperation of researchers from engineering, business administration, and socio-economics as well as active exchange with the other SRAs to integrate data and results. Challenges result from the broad system boundary, the integration of the hierarchy device – process (path) – supply chain in sufficient accuracy, and the consideration of interconnections by transportation and storage of chemical energy carriers and platform chemicals. This cross-sectorial, hierarchical model lays the foundation for the integration of measures against uncertainties and systemic risks, stakeholder perspectives and policy design (see below) to design

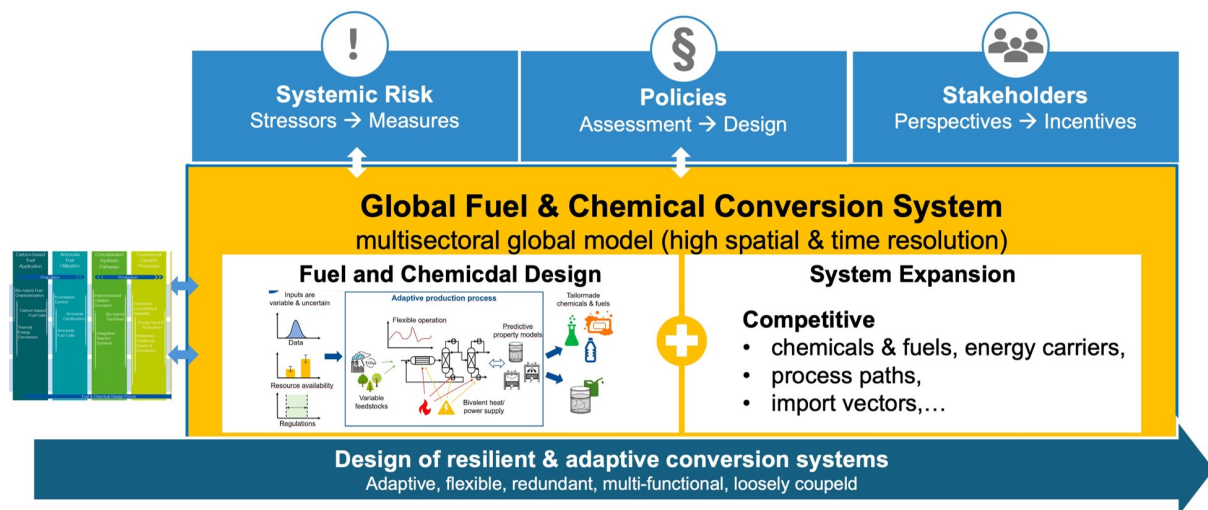


Figure 38: Design of resilient and adaptive conversion systems by integration of stakeholders' incentives, policy design, and systemic risk measures

resilient and adaptive fuel and chemical conversion systems.

An **ex-ante systemic risk measurement and communication approach** is developed to account for the significant (geo-)political, technical, economic, environmental, natural, and social perceptions as well as risks that go along with the installation of global renewable fuel and chemical conversion systems, e. g., [313]. Our approach replaces the often segmented and isolated assessment of stressors, uncertainties and risks of single technologies, fuels or countries by a more complex systemic risk landscape (*Walther, supported by Venghaus*) identifying and prioritizing stressors and risks, and determining interrelations between them. This is accompanied by an assessment of the perception of systemic risks [314] deriving social perception dimensions (e. g., financial or environmental risks, acceptance requirements, energy justice), trade-offs and thresholds of risk, mental models for processing risk information and risk perception levels of stakeholders, statistically segmented risk profiles, and models for risk perception prediction (*Arning, Ziefle*). Based on these results, a risk communication framework (*Arning, supported by Venghaus, Walther & Ziefle*) is developed tailored to address the complex and systemic nature of risks and regarding individual factors such as dual-route information processing, varying levels of trust and expertise in a increasingly complex media and information context.

Stakeholders' (consumers, investors, policymakers) targets, perceptions and decision-models significantly impact market and technology diffusion and system translation [173, 174]. Thus, we overcome the centralized perspective that omits stakeholder-specific decisions, e. g. [298, 304], and analyse stakeholders' roles, claims and positions in the value chain, objectives, constraints, perceptions, and risks using social empirical research, (social) network analysis, data mining, and ML (*Walther, Venghaus, supported by Arning*). This allows to derive **stakeholder-specific decision models**. The behavior and interrelations between stakeholders are analyzed using ML-supported agent-based simulation. The interrelation between overall system's development and stakeholder decisions is done with bilevel optimization, with the upper level representing

the overall fuel and chemical conversion system, and the lower level representing the specific business models of stakeholders. Analyzing the underlying non-cooperative relationship allows to determine the most influencing factors and promising (legal) incentives and policies for stakeholders' as well as overall system's development, trade-offs, synergies and contradictions between the two levels.

For the *ex-ante policy analysis and design* (Venghaus, supported by Walther), a policy monitoring dashboard is developed including both historic as well as current and emerging policy changes with their impact on the conversion system decomposed by sector, technology, product, and type of policy measure. Innovative reverse policy assessment is carried out to determine how market developments and technological innovation impact policy design and policy adaptation. Herein, policy will no longer be considered as an external controlling parameter, but shaped by a proactive policy design approach that is integrated with system design to achieve policy coherence as a prerequisite for the transformation towards a resilient fuel and chemical conversion system.

Finally, results of the systemic risk assessment, stakeholder decisions, policy analysis, and FCDP are merged towards a design framework for *resilient and adaptive fuel and chemical conversion systems*. This relevant task is supported by a Junior Research Group on "AI/ML Data driven System analysis and Modelling". The system will fulfill relevant *resilience criteria* (e.g., redundancy, diversity, optionality, multi-functionality, flexibility, loose coupling, and adaptivity) that are derived, classified and characterized merging knowledge from different disciplines like ecology, engineering, control theory, supply chain management, or energy systems analysis. Complex-dynamic cause-and-effect relations are derived regarding intended and unintended effects, short- and long-term impacts, feedback loops, and delays among system's components with partial differential equation model (Venghaus, Walther). This allows insights in how the system behavior evolves in response to disturbances or changes, and provides a qualitative understanding of resilience dynamics. Results are then aggregated and fed into a prescriptive optimization model for the design of resilient fuel and chemical conversion systems. In this model, resilience criteria, risks, and stochastic uncertainties are integrated into the objective, or modeled as a constraint, a probability or a (worst-case) scenario. We built on the modeling framework in the FCDP that allows to integrate stochastic and robust optimization (Mitsos, Walther). The model enables to determine the impact of resilience measures on the strategic design of fuel and chemical supply chains, determine resilient solutions like (combinations of) redundant capacities, robust location decisions, substitute energy carriers, diversified resources, enhanced facility fortifications, or (short- and long-term) energy storage.

4.5.5.3 Sustainability Assessment

To enable the FSC² vision of "near-to-zero environmental impacts", we assess the environmental impacts of fuels and chemicals with the LCA methodology and also use LCA as objective in our FCDP. While LCA is a standardized and well-established methodology, we have to extend it to fully *capture all environmental and socio-economic impacts and process interactions*

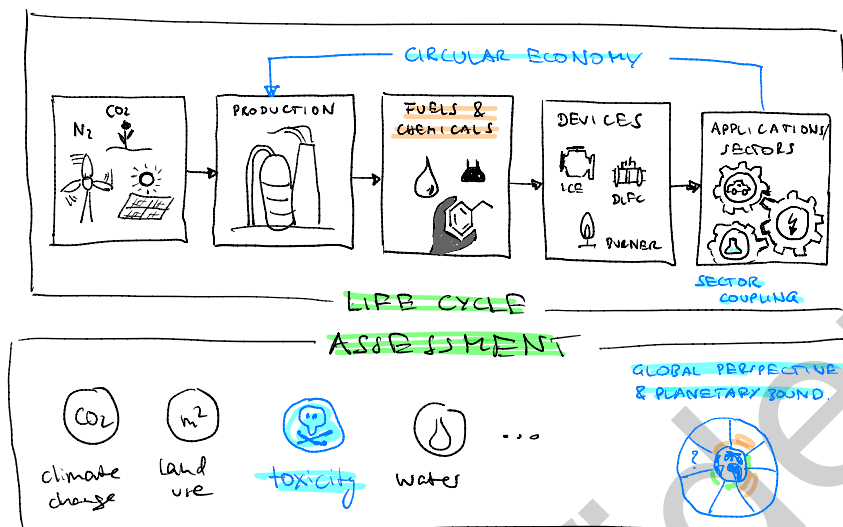


Figure 39: The Sustainability Assessment will cover the entire life-cycle of fuels & chemicals. Methodological extensions are highlighted in blue: toxicity prediction, sector-coupling, planetary boundaries, socio-economic impacts, and circular economy.

holistically, reliably and on a broader scope. Based on LCA, we aim to develop a **Sustainability Assessment** for future fuels & chemicals. For this purpose, we develop improved impact assessment of (eco-)toxicity using novel toxicity predictions for fuel and fuel blends. We broaden the scope from the life cycle of fuels to several sectors (energy, mobility, chemicals) to take into account synergies and competing demands for renewable materials and energy. Further scope extensions are to advance from the impact quantification for fuels (e. g., impacts per MJ of fuel) or mobility services (e. g., impacts per person-km) towards the absolute environmental sustainability defined by the planetary boundaries, and to advance from assessment in individual years and scenarios to an optimization of transition pathways. For chemicals, a life-cycle wide circularity assessment will incorporate anthropogenic stock changes, secondary resource availability and quality aspects. In all approaches, we develop new methods to systematically consider uncertainties and disruptions to improve the reliability and resilience of sustainable fuels.

The methodological research will be accompanied by the application of investigated chemical conversion systems, e. g., ammonia synthesis, integrated CO₂ capture and conversion, and direct-liquid fuel cells. A small and frequent feedback loop with researchers from the other SRAs will guarantee that technologies are developed not only for efficiency, resilience and adaptability, but also for maximum sustainability.

Current State of Research and Previous Work

The [LCA methodology has already been successfully applied and extended](#) in FSC as well as in individual projects by the (new) PIs. In FSC, the blend ketone-esters-alcohol-alkanes (KEAA) has been identified as promising fuel candidate from a holistic perspective. As our reference candidate for a bio-hybrid fuel, KEAA was thoroughly assessed in a toxicity assessment and in a comprehensive LCA study [5].

Major gaps in [toxicity assessment](#) of fuels & chemicals within LCA are the lack of toxicity data, the assessment of mixture toxicity as well as toxicity integration into the LCA framework with harmonized impact indicators [315]. Therefore, Backhaus et al. recently developed an AI-based toolbox for in-silico assessment of the ecotoxicity of chemicals [316, 317]. This toolbox will bridge data gaps encountered when performing LCA-based impact assessment of novel, typically data-poor molecules. Backhaus et al. have also contributed to the harmonization of LCA-based impact indicators [318]. Furthermore, as we continue to expect to obtain fuel blends (such as KEAA) in FSC², the assessment of mixture toxicity is important. In addition to experimental toxicity assessment within FSC, Backhaus et al. have assessed approaches for toxicity prediction for mixtures [319]. LCA has been applied to chemical conversion systems on a molecular and process scale to [guide catalyst design and electrochemical synthesis](#) [221, 222]. As core concept of FSC, the fuel design aims at identifying optimal fuels, also in terms of environmental impacts that can be evaluated with LCA. However, LCA covers multiple environmental impacts. Therefore, in a combined PNFA-based fuel design with LCA as additional optimization objectives, we have performed a [dimensionality reduction to identify the most relevant environmental impacts for bio-hybrid fuels](#) [177]. For the bio-hybrid fuel design for spark-ignition engines, we identified land use and resource use of minerals and metals as key environmental objectives in addition to production cost.

The [flexibility of conversion systems](#) plays a key role for the resilience and adaptability of chemical and energy conversion systems. Therefore, we have developed approaches to enable a fair assessment of industrial demand-side management (DSM) [223] and to evaluate whether and how DSM offers environmental benefit [224, 225]. While LCA typically assumes a static or steady-state approach, we have started developing a [dynamic-prospective LCA using time-explicit inventories](#) to be able to assess multiple time-relevant aspects including process flexibility or systemic transition pathways [226]. For a [circular economy of chemicals](#), it is important to consider the temporal aspects of material flows and anthropogenic material stocks to assess the availability of secondary materials as well as their quality. We have already developed an environmental assessment framework for circular products [227, 228] and systematically reviewed product quality aspects for waste recycling within LCA [229].

We have worked on approaches to [assess LCA impacts on a global scale](#). In a case study for the e-fuel OME3-5, we have analyzed on a European scale whether it is beneficial to use a scarce e-fuels as blend in a fleet or as pure fuel for just a few cars [178]. The combination of experimental data on exhaust emissions and LCA on this broader scale identified that OME3-5 blends are environmentally favorable since already small amounts can reduce NO_x and soot

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emissions efficiently. To assess the absolute environmental sustainability of fuels & chemicals, the LCA approach should be extended from the product-centric assessment of '1 MJ fuel' or '1kg chemical' towards a sector's impact with respect to the planetary boundaries. We have [combined LCA and the planetary boundaries concept](#) together with a design approach for energy systems [230], which is currently adapted for fuels and mobility systems. The socio-economic impacts with respect to a water-energy-food nexus have been analyzed for bio-fuels [320]. An integrated sustainability assessment would be desirable that combines the planetary boundaries framework with socio-economic impacts; however, such combination is still missing.

Objectives

The methodology of LCA will be extended in order to better analyze the full range of sustainability impacts of fuels & chemicals and to optimize them accordingly. For this purpose, we aim to improve LCA-applicable methods for [\(eco-\)toxicity assessment](#) of chemicals, fuels and fuel blends by bridging data gaps via in-silico prediction tools. We will integrate fuel & chemical conversion systems into a [LCA-based, sector-coupled energy system model](#) to reflect [resilience and flexibility as well as synergies and competition between sectors](#). We want to develop new methods to optimize the transition from the current mobility and energy systems towards an absolute sustainable future within [planetary boundaries](#). The LCA methodology and planetary boundaries concept should be extended for [socio-political implications](#) for vital resources such as the water, energy and food nexus. We also aim to integrate [circular economy aspects into the Sustainability Assessment](#) to account for anthropogenic stock changes and product quality.

Work Program

The common approach in this sub-SRA is to develop and apply a LCA-based Sustainability Assessment methodology for fuel & chemical conversion systems. The application will be carried out in close collaboration with the other SRAs for exchange of (experimental or simulation) data as input and assessment results as output to steer further technological research. For example, we will use Sustainability Assessment to identify the environmentally and technically most promising application areas of DLFCs (see Sections 4.5.1.3 & 4.5.2.2). Simultaneously, we will conduct research on the Sustainability Assessment methodology itself for its further advancement. The description of the work program will focus in the methodological assessment advancements and can be classified as follows: (i) improving data availability and quality (inventory data via integration of process models from sub-SRA Fuel & Chemical Design), (ii) improving impact assessment (toxicity assessment and prediction, planetary boundaries assessment, socio-economic impacts within the water-energy-food nexus), and (iii) extending the assessment scope from product to sectors (sector-coupled models for flexible processes and transition pathways, circular economy, scenarios and supply chains from sub-SRA System Integration).

[Improving Data Availability and Quality](#). Experimental results from SRA 1–4 together with process data and models as well as optimization approaches from sub-SRA Fuel & Chemical De-

sign will form the basis for the LCA assessment and LCA-based optimization (Greiff, Mitsos, von der Aßen, Walther). LCA experience shows that data exchange should always be accompanied with a personal explanation and discussion. Here, we can build upon the successful interdisciplinary research of the previous clusters.

Novel Impact Assessment Methods. While the core concept of LCA has always been a holistic approach to avoid burden shifting between life-cycle phases or between environmental impacts, there is still research needed to improve the reliable quantification of environmental impacts such as (eco-)toxicity, and to extend the methodology to socio-economic impacts to assess all dimensions of sustainability. We will improve the comparative toxicological and ecotoxicological LCA-based impact assessments of different fuel types, blends and chemicals (Backhaus). In particular, we will develop and transfer validated mixture assessments from chemical risk assessment to LCA. We will establish suitable indicators for impacts on terrestrial ecosystems, marine ecosystems and groundwater ecosystems that are missing so far. To bridge data gaps, we will implement AI-based in-silico methods to predict (eco-)toxicological impacts and subsequently identify relevant parameters that either should be optimized in fuel & chemical design or that need high-quality empirical data to refine prediction. Overall, uncertainty of impact quantification as well as sensitivity assessment of current environmental footprinting approaches (e. g. as outlined in EU recommendation 2021/9332) will be analyzed.

Current impact assessment results are contextualized via comparisons or normalization. However, whether a fuel or chemical is absolutely sustainable cannot be answered. For the purpose of an absolute environmental sustainability assessment (AESA), we will develop a method by integrated LCA and planetary boundaries (von der Aßen), and apply it to the fuel & chemical supply chain transition (von der Aßen, Walther). We will extend existing AESA approaches to be able to assess transitioning systems rather than a selected reference year (transition pathways rather than “snapshots in time”; see Scope Extension).

The concept of planetary boundaries focuses mostly on impacts caused by emissions, i.e. outputs of human activities, and defines upper limits that should not be exceeded. While the input side is taken into account in traditional LCA via use and depletion of resources, there is also the so-called doughnut economics approach that defines social limits not be exceeded. We will investigate the water-energy-food nexus from a social science perspective including political and cultural dimensions and questions of global justice (Leicht-Scholten).

Scope Extension: from products to sectors to circularity. Synergies as well as competition in the supply chain and production processes suggest to extend the scope from individual products to several sectors, e. g. we simultaneously consider the demand from the mobility, chemical and energy industry (von der Aßen, Walther). For this purpose, we can use our LCA-based, multi-sector energy system design model SecMOD. SecMOD already allows the computation of cost- and GHG-optimal transition pathways until mid-century; however, the focus has so far been on assessing sector-coupling on a broader level. We will incorporate the production processes and supply chains identified within FSC into SecMOD, as well as include other indicators from sub-SRA System Integration. Similarly to sector-coupling, re-use, re-cycling or other kinds of

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circulation cannot be adequately answered on a single product, process or material level and larger scales, e. g. sectoral or economy wide scales, are needed. For recycling for example, anthropogenic stocks, their availability at the end-of-life as well as the quality of secondary material have to be taken into account. For this purpose, we will couple LCA with material flow analysis (MFA) (Greiff).

4.5.5.4 Proposed Staff and Funding of SRA-RACS

Table 4.5.5.1: Proposed Staff in SRA-RACS

Staff category	2026	2027	2028	2029	2030	2031	2032
Postdoctoral researchers	3	3	3	3	3	3	3
Doctoral researchers	12	12	12	12	12	12	12

Table 4.5.5.2: Funding Request for SRA-RACS

Funding category	2026	2027	2028	2029	2030	2031	2032
Staff (Total for 4.5.5)	1121	1143	1166	1189	1213	1237	1262
Direct project costs (excluding staff)	180	180	180	180	180	180	180

4.6 Bibliography

TMFB/FSC publications

- [1] Leitner W, Klankermayer J, Pischinger S et al. Advanced biofuels and beyond: Chemistry solutions for propulsion and production. *Angewandte Chemie (International ed in English)* 2017; 56(20): 5412–5452. DOI:10.1002/anie.201607257.
- [2] Deutz S, Bongartz D, Heuser B et al. Cleaner production of cleaner fuels: wind-to-wheel – environmental assessment of co₂-based oxymethylene ether as a drop-in fuel. *Energy & Environmental Science* 2018; 11(2): 331–343. DOI: 10.1039/C7EE01657C.
- [3] Hellmuth M, Chen B, Bariki C et al. A comparative study on the combustion chemistry of two bio-hybrid fuels: 1,3-dioxane and 1,3-dioxolane. *The journal of physical chemistry A* 2023; 127(1): 286–299. DOI:10.1021/acs.jpca.2c06576).
- [4] Völker S, Groll N, Bachmann M et al. Towards carbon-neutral and clean combustion with hydroformylated fischer-tropsch (hyfit) fuels: Accepted. *NENERGY-23112599* ; DOI:10.1038/s41560-024-01581-z.
- [5] Ackermann P, Braun KE, Burkardt P et al. Designed to be green, economic, and efficient: A ketone-ester-alcohol-alkane blend for future spark-ignition engines. *ChemSusChem* 2021; 14(23): 5254–5264. DOI:10.1002/cssc.202101704.
- [6] Burkardt P, Fleischmann M, Wegmann T et al. On the use of active pre-chambers and bio-hybrid fuels in internal combustion engines. *Energy, Environment, and Sustainability* 2022; : 205–231 DOI:10.1007/978-981-16-8717-4.
- [7] Honecker C, Lehrheuer B, Pischinger S et al. Molecularly-controlled high swirl combustion system for ethanol/1-octanol dual fuel combustion. *Fuel* 2023; 345. DOI:10.1016/j.fuel.2023.128184.
- [8] Tripathi R, Burke U, Ramalingam AK et al. Oxidation of 2-methylfuran and 2-methylfuran/n-heptane blends: An experimental and modeling study. *Combustion and Flame* 2018; 196: 54–70. DOI:10.1016/j.combustflame.2018.05.032.
- [9] Cai L, Minwegen H, Kruse S et al. Exploring the combustion chemistry of a novel lignocellulose-derived biofuel: cyclopentanol. part ii: experiment, model validation, and functional group analysis. *Combustion and Flame* 2019; 210: 134–144. DOI:10.1016/j.combustflame.2019.08.025.
- [10] Morsch P, Döntgen M and Heufer KA. Kinetic investigations on the high- and low-temperature chemistry of ethyl acetate. *Combustion and Flame* 2022; 243. DOI:10.1016/j.combustflame.2022.111995.
- [11] Wildenberg A, Döntgen M, Roy IS et al. Solving the riddle of the high-temperature chemistry of 1,3-dioxolane. *Proceedings of the Combustion Institute* 2023; 39(1): 705–713. DOI:10.1016/j.proci.2022.07.194.
- [12] Morsch P, Fenard Y and Heufer KA. Comparative study on ethyl butanoate reactivity - experimental investigation and kinetic modeling of the c6ethyl ester. *Proceedings of the Combustion Institute* 2021; 38(1): 939–946. DOI: 10.1016/j.proci.2020.06.246.

- [13] Döntgen M, Przybylski-Freund MD, Kröger LC et al. Automated discovery of reaction pathways, rate constants, and transition states using reactive molecular dynamics simulations. *Journal of Chemical Theory and Computation* 2015; 11(6): 2517–2524. DOI:10.1021/acs.jctc.5b00201.
- [14] Chair I, Kopp W, Leonhard K et al. Chemtrayzer, 2024. DOI:10.5281/ZENODO.10954962.
- [15] Döntgen M, Schmalz F, Kopp WA et al. Automated chemical kinetic modeling via hybrid reactive molecular dynamics and quantum chemistry simulations. *Journal of Chemical Information and Modeling* 2018; 58(7): 1343–1355. DOI: 10.1021/acs.jcim.8b00078.
- [16] Minwegen H, Döntgen M, Fenard Y et al. Proceeding on the riddles of ketene pyrolysis by applying ab initio quantum chemical computational methods in a detailed kinetic modeling study. *Proceedings of the Combustion Institute* 2021; 38(1): 749–755. DOI:10.1016/j.proci.2020.08.046.
- [17] Döntgen M, Kopp WA, vom Lehn F et al. Updated thermochemistry for renewable transportation fuels: New groups and group values for acetals and ethers, their radicals, and peroxy species. *International Journal of Chemical Kinetics* 2021; 53(2): 299–307. DOI:10.1002/kin.21443.
- [18] vom Lehn F, Cai L and Pitsch HG. Iterative model-based experimental design for efficient uncertainty minimization of chemical mechanisms. *[38th International Symposium on Combustion]*; 2/11 2021; .
- [19] Wildenberg A, Fenard Y, Carbonnier M et al. An experimental and kinetic modeling study on the oxidation of 1,3-dioxolane. *Proceedings of the Combustion Institute* 2021; 38(1): 543–553. DOI:10.1016/j.proci.2020.06.362.
- [20] Hellmuth M, Cameron F, Faller S et al. Synergistic effect on pah and soot formation in ethylene counterflow diffusion flames by the addition of 1,3-dioxolane - a bio-hybrid fuel. *Proceedings of the Combustion Institute* 2023; 39(1): 899–908. DOI:10.1016/j.proci.2022.07.164.
- [21] Cameron F, Ren Y, Girhe S et al. In-situ laser diagnostic and numerical investigations of soot formation characteristics in ethylene and acetylene counterflow diffusion flames blended with dimethyl carbonate and methyl formate. *Proceedings of the Combustion Institute* 2023; 39(1): 1109–1118. DOI:10.1016/j.proci.2022.07.219.
- [22] vom Lehn F, Cai L and Pitsch HG. Iterative model-based experimental design for efficient uncertainty minimization of chemical mechanisms. *Proceedings of the Combustion Institute* 2021; 38(1): 1033–1042. DOI:10.1016/j.proci.2020.06.188.
- [23] Girhe S, Snackers A, Lehmann T et al. Comprehensive quantitative assessment and improvements of ammonia and ammonia/hydrogen combustion kinetic models. *Combustion and Flame* 2024; : Submitted.
- [24] Wu X, Fischer M, Nolte A et al. Perovskite catalyst for in-cylinder coating to reduce raw pollutant emissions of internal combustion engines. *ACS omega* 2022; 7(6): 5340–5349. DOI:10.1021/acsomega.1c06530.
- [25] Breuer M and Heufer KA. Consistent global modeling approach for the autoignition of linear alkanes. In *11th European Combustion Meeting 2023: April 26-28, 2023, Rouen, France: proceedings / organised by CORIA UMR 6614 and French Section Combustion Institute*. Rouen: French Section Combustion Institute, pp. 1–6.
- [26] Döntgen M, Eckart S, Fritsche C et al. Experimental and chemical kinetic modeling study of trimethoxy methane combustion. *Proceedings of the Combustion Institute* 2023; 39(1): 305–314. DOI:10.1016/j.proci.2022.09.023.
- [27] Morsch P, Döntgen M and Heufer KA. High- and low-temperature ignition delay time study and modeling efforts on vinyl acetate. *Proceedings of the Combustion Institute* 2023; 39(1): 115–123. DOI:10.1016/j.proci.2022.07.058.
- [28] Döntgen M, Wildenberg A and Heufer KA. Laser absorption shock tube study of c1 to c4 n-alkyl formate pyrolysis: (submitted). *Proceedings of the Combustion Institute* 2024; .
- [29] Burkardt P, Wouters C and Pischinger S. Evaluation of pre-chamber orifice orientation in an ethanol-fueled spark-ignition engine for passenger car applications. *SAE International Journal of Engines* 2021; 15(4). DOI:10.4271/03-15-04-0024.
- [30] Burkardt P, Wouters C and Pischinger S. Potential of alcohol fuels in active and passive pre-chamber applications in a passenger car spark-ignition engine. *International Journal of Engine Research* 2023; 24(2): 494–505. DOI: 10.1177/14680874211053168.
- [31] Burkardt P, Wouters C and Pischinger S. Beating neat fuels by dedicated blending: Performance analysis of bio-hybrid fuel blends on a spark-ignition engine for passenger car applications. *Fuel* 2023; 331. DOI:10.1016/j.fuel.2022.125579.
- [32] Burkardt P, Ottenwälder T, König A et al. Toward co-optimization of renewable fuel blend production and combustion in ultra-high efficiency si engines. *International Journal of Engine Research* 2023; 24(1): 29–41. DOI:10.1177/14680874211040995.
- [33] Grütering C, Honecker C, Hofmeister M et al. Methyl ketones: a comprehensive study of a novel biofuel. *Sustainable Energy & Fuels* 2024; DOI:10.1039/D4SE00035H.
- [34] Dewor R, Fleischmann M, Brands T et al. Resolving the combustion zones of bio-hybrid fuels in reactivity controlled compression ignition combustion using tracer-activated luminescence imaging. *SAE International Journal of Fuels and Lubricants* 2022; 16(1). DOI:10.4271/04-16-01-0004.
- [35] Wegmann T, Meinke M, Fleischmann M et al. (eds.). *SAE Technical Paper Series*. SAE Technical Paper Series, SAE International400 Commonwealth Drive, Warrendale, PA, United States, 2024.
- [36] Fleischmann M, Burkardt P, Wegmann T et al. Optical investigation of methanol fueled active pre-chamber applications for internal combustion engines, 10.-12.05.2022.
- [37] Röhrens D, Abouserie A, Wang B et al. Microwave-assisted co oxidation over perovskites as a model reaction for exhaust aftertreatment—a critical assessment of opportunities and challenges. *Catalysts* 2022; 12(7). DOI:10.3390/catal12070802.
- [38] Bardow A, Voelker S, Groll N et al. *Towards carbon-neutral and clean combustion with hydroformylated Fischer-Tropsch (HyFIT) fuels*. 2023. DOI:10.21203/rs.3.rs-3686247/v1.

4 Research Program

- [39] Hofmeister M, Frische A, Grunewald MME et al. Tribological properties of ptfе sealing materials with regard to bio-hybrid fuels. In *Sealing technology - old school and cutting edge : International Sealing Conference : 21st ISC, Stuttgart, Germany, October 12-13, 2022 / eine Kooperation von IMA, Uni Stuttgart; VDMA Fluidtechnik*. Frankfurt am Main: Fachverband Fluidtechnik im VDMA e.V, pp. 89–104.
- [40] Hofmeister M, Laker J, Fischer M et al. Neue herausforderungen an dichtungswerkstoffe im hinblick auf bio-hybride kraftstoffe. *Mobility : mobile Lösungen für den betrieblichen Einsatz* 2022; 7: 44–48.
- [41] Wouters C, Lehrheuer B, Pischinger S et al. Evaluation of synthetic gasoline fuels and alcohol blends in a spark-ignition engine. *SAE International Journal of Fuels and Lubricants* 2022; 15(3). DOI:10.4271/04-15-03-0017.
- [42] Schnepf Z, Thomas M, Glatzel S et al. One pot route to sponge-like fe₃n nanostructures. *Journal of Materials Chemistry* 2011; 21(44): 17760. DOI:10.1039/c1jm12842f.
- [43] Glaznev R, Schwenzer C, Hesse R et al. Ultra-slow ammonia flame speeds - a microgravity study on radiation. *Submitted to Proceedings of the Combustion Institute* 2024; .
- [44] Zhu Y, Curran HJ, Girhe S et al. The combustion chemistry of ammonia and ammonia/hydrogen mixtures: A comprehensive chemical kinetic modeling study. *Combustion and Flame* 2024; 260: 113239. DOI:10.1016/j.combustflame.2023.113239.
- [45] Slabaugh CD, Boxx I, Werner S et al. Structure and dynamics of premixed swirl flames at elevated power density. *AIAA Journal* 2016; 54(3): 946–961. DOI:10.2514/1.J054294.
- [46] Dennis CN, Slabaugh CD, Boxx IG et al. Chirped probe pulse femtosecond coherent anti-stokes raman scattering thermometry at 5 khz in a gas turbine model combustor. *Proc Combust Inst* 2015; 35(3): 3731–3738. DOI:10.1016/j.proci.2014.06.063.
- [47] Wu Z, Jiang D, Wang J et al. Knowledge-based bert: a method to extract molecular features like computational chemists. *Briefings in bioinformatics* 2022; 23(3). DOI:10.1093/bib/bbac131.
- [48] Kirsch V, Hermans M, Schönberger J et al. Transparent high-pressure nozzles for visualization of nozzle internal and external flow phenomena. *The Review of scientific instruments* 2019; 90(3): 033702. DOI:10.1063/1.5065658.
- [49] Saha A, Deshmukh AY, Grenga T et al. Dimensional analysis of vapor bubble growth considering bubble–bubble interactions in flash boiling microdroplets of highly volatile liquid electrofuels. *International Journal of Multiphase Flow* 2023; 165. DOI: 10.1016/j.ijmultiphaseflow.2023.104479.
- [50] Wegmann T, Meinke M, Fleischmann M et al. Numerical analysis of mixing of bio-hybrid fuels in a direct injection engine with a pre-chamber ignition system. In Wegmann T, Meinke M, Fleischmann M et al. (eds.) *SAE Technical Paper Series*. SAE Technical Paper Series, SAE International400 Commonwealth Drive, Warrendale, PA, United States. DOI: 10.4271/2024-01-2619.
- [51] Tchoupe E, Lauwers D, Heidemanns L et al. Optical in situ analysis of gas bubble evolution in electrochemical machining based on similarity theory using particle image velocimetry. *Procedia CIRP* 2023; 117: 257–262. DOI: 10.1016/j.procir.2023.03.044.
- [52] Schönberger Alvarez AA, Özyalcin C, Padeken T et al. Impact of unintentionally formed ch₂o in oxygenated fuel exhausts on denox-scr at different no₂/nox ratios under close to real conditions. *Catalysis Science & Technology* 2023; 13(14): 4069–4081. DOI:10.1039/d2cy01935c.
- [53] Simböck J, Ghiasi M, Schönebaum S et al. Electronic parameters in cobalt-based perovskite-type oxides as descriptors for chemocatalytic reactions. *Nature communications* 2020; 11(1): 652. DOI:10.1038/s41467-020-14305-0.
- [54] Lei H, Chen D, Yang JY et al. Revealing the formation and reactivity of cage-confined cu pairs in catalytic nox reduction over cu-ssz-13 zeolites by in situ uv-vis spectroscopy and time-dependent dft calculation. *Environmental Science & Technology* 2023; 57(33): 12465–12475. DOI:10.1021/acs.est.3c00458.
- [55] Chen B, Liu P, Pelucchi M et al. New insights into the oxidation chemistry of pyrrole, an n-containing biomass tar component. *Proceedings of the Combustion Institute* 2023; 39(1): 73–84. DOI:10.1016/j.proci.2022.07.019.
- [56] Yadav G and Khetan A. First principles energetic span analysis of the activity of transition metal catalysts for n₂o decomposition: The reversal of descriptor roles in the presence of no. *Catalysis Today* 2024; : 114892DOI: 10.1016/j.cattod.2024.114892.
- [57] Zimmerman JB, Anastas PT, Erythropel HC et al. Designing for a green chemistry future. *Science* 2020; 367(6476): 397–400. DOI:10.1126/science.aay3060.
- [58] Schieweck BG, Westhues NF and Klankermayer J. A highly active non-precious transition metal catalyst for the hydrogenation of carbon dioxide to formates. *Chemical science* 2019; 10(26): 6519–6523. DOI:10.1039/c8sc05230a.
- [59] Vennewald M, Sackers NM, Lemhoff A et al. Dynamics of palladium single-atoms on graphitic carbon nitride during ethylene hydrogenation. *Journal of Catalysis* 2023; 421: 134–144. DOI:10.1016/j.jcat.2023.03.011.
- [60] Beydoun K and Klankermayer J. Ruthenium-catalyzed synthesis of cyclic and linear acetals by the combined utilization of co₂, h₂, and biomass derived diols. *Chemistry – A European Journal* 2019; 25(49): 11412–11415. DOI: 10.1002/chem.201901660.
- [61] Spöring JD, Wiesenthal J, Pfennig VS et al. Effective production of selected dioxolanes by sequential bio- and chemocatalysis enabled by adapted solvent switching. *ChemSusChem* 2023; 16(2): e202201981. DOI:10.1002/cssc.202201981).
- [62] Jeske K, Rösler T, Belleflamme M et al. Direct conversion of syngas to higher alcohols via tandem integration of fischer–tropsch synthesis and reductive hydroformylation. *Angewandte Chemie* 2022; 134(31). DOI:10.1002/ange.202201004.
- [63] Jüring-Will P, Botz T, Franciò G et al. A "power-to-x" route to acetic acid via palladium-catalyzed isomerization of methyl formate. *ChemSusChem* 2022; 15(16): e202201006. DOI:10.1002/cssc.202201006.

- [64] Liebal UW, Blank LM and Ebert BE. Co₂ to succinic acid - estimating the potential of biocatalytic routes. *Metabolic engineering communications* 2018; 7: e00075. DOI:10.1016/j.mec.2018.e00075.
- [65] Ullmann L, Phan ANT, Kaplan DKP et al. Ustilaginaceae biocatalyst for co-metabolism of co₂-derived substrates toward carbon-neutral itaconate production. *J. fungi* 2021, 7, 98, 2021.
- [66] Jovanovic S, Jakes P, Merz S et al. In operando nmr investigations of the aqueous electrolyte chemistry during electrolytic co₂ reduction. *Communications chemistry* 2023; 6(1): 268. DOI:10.1038/s42004-023-01065-3.
- [67] Cramer HH, Chatterjee B, Weyhermüller T et al. Controlling the product platform of carbon dioxide reduction: Adaptive catalytic hydrosilylation of co₂ using a molecular cobalt(ii) triazine complex. *Angewandte Chemie (International ed in English)* 2020; 59(36): 15674–15681. DOI:10.1002/anie.202004463.
- [68] Musialek SD, Pfänder N and Palkovits R. Bimetallic ptcu/c catalysts for glycerol assisted hydrogen evolution in acidic media. *ChemElectroChem* 2023; DOI:10.1002/celec.202300193.
- [69] Mürtz SD, Musialek F, Pfänder N et al. Bimetallic ptcu/c catalysts for glycerol assisted hydrogen evolution in acidic media. *ChemElectroChem* 2023; 10(11). DOI:10.1002/celec.202201114.
- [70] Haus MO, Winter B, Fleitmann L et al. Making more from bio-based platforms: life cycle assessment and techno-economic analysis of n-vinyl-2-pyrrolidone from succinic acid. *Green Chemistry* 2022; 24(17): 6671–6684. DOI: 10.1039/D2GC01219G.
- [71] Nattermann M, Wenk S, Pfister P et al. Engineering a new-to-nature cascade for phosphate-dependent formate to formaldehyde conversion in vitro and in vivo. *Nature communications* 2023; 14(1): 2682. DOI:10.1038/s41467-023-38072-w.
- [72] Kaithal A, Hölscher M and Leitner W. Carbon monoxide and hydrogen (syngas) as a c1-building block for selective catalytic methylation. *Chemical Science* 2020; 12(3): 976–982. DOI:10.1039/D0SC05404F.
- [73] Pfennig VS, Vilella RC, Nikodemus J et al. Mechanochemical grignard reactions with gaseous co₂ and sodium methyl carbonate. *Angewandte Chemie (International ed in English)* 2022; 61(9): e202116514. DOI:10.1002/anie.202116514.
- [74] Fricke C, Sperger T, Mendel M et al. Catalysis with palladium(i) dimers. *Angewandte Chemie International Edition* 2021; 60(7): 3355–3366. DOI:10.1002/anie.202011825.
- [75] Kapat A, Sperger T, Guven S et al. E-olefins through intramolecular radical relocation. *Science (New York, NY)* 2019; 363(6425): 391–396. DOI:10.1126/science.aav1610.
- [76] Dahiya A, Schoetz MD and Schoenebeck F. Orthogonal olefination with organogermanes. *Angewandte Chemie* 2023; 135(43). DOI:10.1002/ange.202310380.
- [77] Scattolin T, Bouayad-Gervais S and Schoenebeck F. Straightforward access to n-trifluoromethyl amides, carbamates, thiocarbamates and ureas. *Nature* 2019; 573(7772): 102–107. DOI:10.1038/s41586-019-1518-3.
- [78] Hueffel JA, Sperger T, Funes-Ardoiz I et al. Accelerated dinuclear palladium catalyst identification through unsupervised machine learning. *Science* 2021; 374(6571): 1134–1140. DOI:10.1126/science.abj0999.
- [79] Karl TM, Bouayad-Gervais S, Hueffel JA et al. Machine learning-guided development of trialkylphosphine ni(i) dimers and applications in site-selective catalysis. *Journal of the American Chemical Society* 2023; 145(28): 15414–15424. DOI: 10.1021/jacs.3c03403.
- [80] Szymanski NJ, Rendy B, Fei Y et al. An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* 2023; 624(7990): 86–91. DOI:10.1038/s41586-023-06734-w.
- [81] Kalikadien AV, Mirza A, Hossaini AN et al. Paving the road towards automated homogeneous catalyst design. *ChemPlusChem* 2024; : e202300702 DOI:10.1002/cplu.202300702.
- [82] Trunschke A. Prospects and challenges for autonomous catalyst discovery viewed from an experimental perspective. *Catalysis Science & Technology* 2022; 12(11): 3650–3669. DOI:10.1039/D2CY00275B.
- [83] Klemm SO, Topalov AA, Laska CA et al. Coupling of a high throughput microelectrochemical cell with online multielemental trace analysis by icp-ms. *Electrochemistry Communications* 2011; 13(12): 1533–1535. DOI:10.1016/j.elecom.2011.10.017.
- [84] Schuppert AK, Topalov AA, Katsounaros I et al. A scanning flow cell system for fully automated screening of electrocatalyst materials. *Journal of The Electrochemical Society* 2012; 159(11): F670–F675. DOI:10.1149/2.009211jes.
- [85] Röttcher NC, Akkoc GD, Finger S et al. Accelerating materials research with a comprehensive data management tool: a case study on an electrochemical laboratory. *Journal of Materials Chemistry A* 2024; 12(7): 3933–3942. DOI: 10.1039/D3TA06247C.
- [86] Xiu ZL and Zeng AP. Present state and perspective of downstream processing of biologically produced 1,3-propanediol and 2,3-butanediol. *Applied microbiology and biotechnology* 2008; 78(6): 917–926. DOI:10.1007/s00253-008-1387-4.
- [87] Schroer G, Toussaint V, Heyman B et al. Recovery of biobased 2,3-butanediol from fermentation broths by liquid-phase adsorption onto phenylboronate polymers. *Current Research in Green and Sustainable Chemistry* 2022; 5. DOI: 10.1016/j.crgsc.2022.100297.
- [88] Zensen T, Röper T, Fuchs T et al. Porous organic frameworks for preferable adsorption of trans-1,2-diols over cis-1,2-diols. *Applied Materials Today* 2022; 28. DOI:10.1016/j.apmt.2022.101523.
- [89] Mengers HG, von Westarp WG, Brücker D et al. Yeast-based production and in situ purification of acetaldehyde. *Bioprocess and Biosystems Engineering* 2022; 45(4): 761–769. DOI:10.1007/s00449-022-02697-w.
- [90] Spöring JD, Graf von Westarp W, Kipp CR et al. Enzymatic cascade in a simultaneous, one-pot approach with in situ product separation for the asymmetric production of (4 s,5 s)-octanediol. *Organic Process Research and Development* 2022; 26(7): 2038–2045. DOI:10.1021/acs.oprd.1c00433.

4 Research Program

- [91] Martínez-Calvo M and Mascareñas JL. Organometallic catalysis in biological media and living settings. *Coordination Chemistry Reviews* 2018; 359: 57–79. DOI:10.1016/j.ccr.2018.01.011.
- [92] van Schie MMCH, Spöring JD, Bocola M et al. Applied biocatalysis beyond just buffers—from aqueous to unconventional media. options and guidelines. *Green Chemistry* 2021; 23(9): 3191–3206.
- [93] Mohd Azhar SH, Abdulla R, Jambo SA et al. Yeasts in sustainable bioethanol production: A review. *Biochemistry and biophysics reports* 2017; 10: 52–61. DOI:10.1016/j.bbrep.2017.03.003.
- [94] Trost BM. The atom economy—a search for synthetic efficiency. *Science (New York, NY)* 1991; 254(5037): 1471–1477. DOI:10.1126/science.1962206.
- [95] Trost BM. On inventing reactions for atom economy. *Accounts of Chemical Research* 2002; 35(9): 695–705. DOI: 10.1021/ar010068z.
- [96] Guntermann N, Mengers HG, Franciò G et al. Bio-energy conversion with carbon capture and utilization (beccu): Integrated biomass fermentation and chemo-catalytic co₂hydrogenation for bioethanol and formic acid co-production. *Green Chemistry* 2021; 23(24): 9860–9864. DOI:10.1039/d1gc02915k.
- [97] Xu Y, Isom L and Hanna MA. Adding value to carbon dioxide from ethanol fermentations. *Bioresource Technology* 2010; 101(10): 3311–3319. DOI:10.1016/j.biortech.2010.01.006.
- [98] Mengers HG, Guntermann N, Graf von Westarp W et al. Three sides of the same coin: Combining microbial, enzymatic, and organometallic catalysis for integrated conversion of renewable carbon sources. *Chemie-Ingenieur-Technik* 2023; 95(4): 485–490. DOI:10.1002/cite.202200169.
- [99] von Campenhausen M, Demling P, Bongartz P et al. Novel multiphase loop reactor with improved aeration prevents excessive foaming in rhamnolipid production by *Pseudomonas putida*. *Discover Chemical Engineering* 2023; 3(1). DOI: 10.1007/s43938-023-00018-5.
- [100] Ullmann L, Guntermann N, Kohl P et al. Improved itaconate production with *Ustilago cynodontis* via co-metabolism of co₂-derived formate. *Journal of fungi (Basel, Switzerland)* 2022; 8(12). DOI:10.3390/jof8121277.
- [101] Diehl T, Lanzerath P, Franciò G et al. A self-separating multiphasic system for catalytic hydrogenation of co₂ and co₂-derivatives to methanol. *ChemSusChem* 2022; 15(22): e202201250. DOI:10.1002/cssc.202201250.
- [102] Aigner M, Roth D, Rußkamp J et al. Model-based equipment design for the biphasic production of 5-hydroxymethylfurfural in a tubular reactor. *AIChE Journal* 2020; 66(4). DOI:10.1002/aic.16849.
- [103] Roth DM, Dunkel P, Kampwerth J et al. Beyond partition coefficients: Model-based solvent screening in extractive-reaction processes considering fluid dynamics and mass transfer limitations. *Industrial & Engineering Chemistry Research* 2022; 61(39): 14546–14560. DOI:10.1021/acs.iecr.2c01820.
- [104] Harhues T, Padligur MC, Bertram F et al. Integrated biphasic electrochemical oxidation of hydroxymethylfurfural to 2,5-furandicarboxylic acid. *ACS Sustainable Chemistry and Engineering* 2023; 11(23): 8413–8419. DOI: 10.1021/acssuschemeng.3c01403.
- [105] Grütering C, Harhues T, Speen F et al. Acetoin production by resting cells of *Lactococcus lactis* for direct electrochemical synthesis of 2-butanone. *Green Chemistry* 2023; 25(22): 9218–9225. DOI:10.1039/d3gc02513f.
- [106] Weber N, Linkhorst J, Keller RG et al. Tailoring pore networks – gas diffusion electrodes via additive manufacturing. *Advanced Materials Technologies* 2023; DOI:10.1002/admt.202300720.
- [107] Weber N, Möntmann M, Wessling M et al. A continuous flow reactor for tubular gas diffusion electrodes. *Chemical Engineering Journal* 2024; 486: 150031. DOI:10.1016/j.cej.2024.150031.
- [108] Wiesner F, Limper A, Marth C et al. Additive manufacturing of intertwined electrode pairs - guided mass transport with gyroids. *Advanced Engineering Materials* 2023; 25(1). DOI:10.1002/adem.202200986.
- [109] Limper A, Harhues T, Keller RG et al. Two-level porosity electrodes from metal-polymer dispersions. *Electrochemistry Communications* 2022; 135. DOI:10.1016/j.elecom.2022.107205.
- [110] Padligur MC, Linnartz CJ, Zimmer S et al. Coupled optical-electric monitoring of charge percolation events in carbon flow-electrodes. *Chemical Engineering Journal* 2024; 482: 148749. DOI:10.1016/j.cej.2024.148749.
- [111] Sibirtsev S, Zhai S and Jupke A. Mask r-cnn based droplet detection in liquid–liquid systems, part 3: Model generalization for accurate processing performance independent of image quality. *Chemical Engineering Research and Design* 2024; 202: 161–168. DOI:10.1016/j.cherd.2023.12.005.
- [112] Utomo RNC, Li WJ, Tiso T et al. Defined microbial mixed culture for utilization of polyurethane monomers. *ACS Sustainable Chemistry & Engineering* 2020; 8(47): 17466–17474. DOI:10.1021/acssuschemeng.0c06019.
- [113] Germer A, Tiso T, Müller C et al. Exploiting the natural diversity of rhlA acyltransferases for the synthesis of the rhamnolipid precursor 3-(3-hydroxyalkanoyloxy) alkanolic acid. *Applied and environmental microbiology* 2020; 86(6): e02317–19.
- [114] Meyers J, Mensah JB, Holzhäuser FJ et al. Electrochemical conversion of a bio-derivable hydroxy acid to a drop-in oxygenate diesel fuel. *Energy & Environmental Science* 2019; 12(8): 2406–2411. DOI:10.1039/C9EE01485C.
- [115] Tiso T, Demling P, Karmainski T et al. Foam control in biotechnological processes—challenges and opportunities. *Discover Chemical Engineering* 2024; 4(1). DOI:10.1007/s43938-023-00039-0.
- [116] Schroer G, Deischer J, Zensen T et al. Structure-performance correlations of cross-linked boronic acid polymers as adsorbents for recovery of fructose from glucose–fructose mixtures. *Green Chemistry* 2020; 22(2): 550–562. DOI: 10.1039/C9GC03151K.

- [117] Schroer G. *Gewinnung von biomassebasierten polaren Verbindungen aus Wasser durch Adsorption*. PhD Thesis, Dissertation, RWTH Aachen University, 2021, 2021.
- [118] Hosseinpour Tehrani H, Becker J, Bator I et al. Integrated strain- and process design enable production of 220 g l⁻¹ itaconic acid with *ustilago maydis*. *Biotechnology for biofuels* 2019; 12: 263. DOI:10.1186/s13068-019-1605-6.
- [119] Schlembach I, Hosseinpour Tehrani H, Blank LM et al. Consolidated bioprocessing of cellulose to itaconic acid by a co-culture of *trichoderma reesei* and *ustilago maydis*. *Biotechnology for biofuels* 2020; 13(1): 207. DOI: 10.1186/s13068-020-01835-4.
- [120] Weiermüller J, Akermann A, Laudensack W et al. Brewers' spent grain as carbon source for itaconate production with engineered *ustilago maydis*. *Bioresource Technology* 2021; 336: 125262. DOI:10.1016/j.biortech.2021.125262.
- [121] Pastoors J, Baltin C, Bettmer J et al. Respiration-based investigation of adsorbent-bioprocess compatibility. *Biotechnology for biofuels and bioproducts* 2023; 16(1): 49. DOI:10.1186/s13068-023-02297-0.
- [122] Ullmann L, Wibberg D, Busche T et al. Seventeen *ustilaginaceae* high-quality genome sequences allow phylogenomic analysis and provide insights into secondary metabolite synthesis. *Journal of Fungi* 2022; 8(3). DOI:10.3390/jof8030269.
- [123] Ziegler AL, Ullmann L, Boßmann M et al. Itaconic acid production by co-feeding of *ustilago maydis*: A combined approach of experimental data, design of experiments, and metabolic modeling. *Biotechnology and Bioengineering* 2024; DOI:10.1002/bit.28693.
- [124] Guntermann N, Franciò G and Leitner W. Hydrogenation of co₂ to formic acid in biphasic systems using aqueous solutions of amino acids as the product phase. *Green Chemistry* 2022; 24(20): 8069–8075. DOI:10.1039/d2gc02598a.
- [125] Cramer HH, Das S, Wodrich MD et al. Theory-guided development of homogeneous catalysts for the reduction of co₂ to formate, formaldehyde, and methanol derivatives. *Chemical science* 2023; 14(11): 2799–2807. DOI:10.1039/D2SC06793E.
- [126] Louis Anandaraj SJ, Kang L, DeBeer S et al. Catalytic hydrogenation of co₂ to formate using ruthenium nanoparticles immobilized on supported ionic liquid phases. *Small* 2023; 19(18): e2206806. DOI:10.1002/smll.202206806.
- [127] Püschel S, Störte S, Topphoff J et al. Green process design for reductive hydroformylation of renewable olefin cuts for drop-in diesel fuels. *ChemSusChem* 2021; 14(23): 5226–5234. DOI:10.1002/cssc.202100929.
- [128] Gao W, Liu S, Wang Z et al. Outlook of cobalt-based catalysts for heterogeneous hydroformylation of olefins: From nanostructures to single atoms. *Energy & Fuels* 2024; 38(4): 2526–2547. DOI:10.1021/acs.energyfuels.3c03037.
- [129] Westhues S, Idel J and Klankermayer J. Molecular catalyst systems as key enablers for tailored polyesters and polycarbonate recycling concepts. *Science advances* 2018; 4(8): eaat9669. DOI:10.1126/sciadv.aat9669.
- [130] Beydoun K, Thenert K, Wiesenthal J et al. Utilization of formic acid as c₁ building block for the ruthenium-catalyzed synthesis of formaldehyde surrogates. *ChemCatChem* 2020; 12(7): 1944–1947. DOI:10.1002/cctc.201902332.
- [131] Merchan AL, Fischöder T, Hee J et al. Chemical recycling of bioplastics: technical opportunities to preserve chemical functionality as path towards a circular economy. *Green Chemistry* 2022; 24(24): 9428–9449. DOI:10.1039/d2gc02244c.
- [132] Bordet A, El Sayed S, Sanger M et al. Selectivity control in hydrogenation through adaptive catalysis using ruthenium nanoparticles on a co₂-responsive support. *Nature chemistry* 2021; 13(9): 916–922. DOI:10.1038/s41557-021-00735-w.
- [133] Zhang Y, Tian Z, Huang L et al. Advances in catalytic decomposition of n₂o by noble metal catalysts. *Catalysts* 2023; 13(6): 943. DOI:10.3390/catal13060943.
- [134] Köhnke K, Wessel N, Esteban J et al. Operando monitoring of mechanisms and deactivation of molecular catalysts. *Green Chemistry* 2022; 24(5): 1951–1972. DOI:10.1039/d1gc04383h.
- [135] Fassbach TA, Ji JM, Vorholt AJ et al. Recycling of homogeneous catalysts—basic principles, industrial practice, and guidelines for experiments and evaluation. *ACS Catalysis* 2024; 14(9): 7289–7298. DOI:10.1021/acscatal.4c01006.
- [136] Yang J, Hilpert F, Qiu Y et al. Interactions of the ionic liquid [c₂c₁im][dca] with au(111) electrodes: Interplay between ion adsorption, electrode structure, and stability. *The Journal of Physical Chemistry C* 2024; 128(7): 2834–2843. DOI: 10.1021/acs.jpcc.3c07122.
- [137] Klein M, Troglauer DL and Waldvogel SR. Dehydrogenative imination of low-valent sulfur compounds—fast and scalable synthesis of sulfilimines, sulfenamides, and sulfenimide esters. *JACS Au* 2023; 3(2): 575–583. DOI:10.1021/jacsau.2c00663.
- [138] Rowbotham JS, Nicholson JH, Ramirez MA et al. Biocatalytic reductive amination as a route to isotopically labelled amino acids suitable for analysis of large proteins by nmr. *Chemical Science* 2023; 14(43): 12160–12165. DOI: 10.1039/D3SC01718D.
- [139] Kurig N and Palkovits R. Electrochemical nitration for organic c–n bond formation: a current view on possible n-sources, mechanisms, and technological feasibility. *Green Chemistry* 2023; DOI:10.1039/d3gc02084c.
- [140] Kümper J, Meyers J, Sebers R et al. Electrochemical transformation of d,l-glutamic acid into acrylonitrile. *Green Chemistry* 2023; 25(16): 6231–6237. DOI:10.1039/d3gc01045g.
- [141] Heidarian A, Wehner M, Padligur MC et al. A microfluidic proton flow reactor system: In-situ visualisation of hydrogen evolution and storage in carbon-based slurry electrodes. *Journal of Power Sources* 2023; 569. DOI: 10.1016/j.jpowsour.2023.233026.
- [142] Yan D, Mebrahtu C, Wang S et al. Innovative electrochemical strategies for hydrogen production: From electricity input to electricity output. *Angewandte Chemie (International ed in English)* 2023; 62(16): e202214333. DOI: 10.1002/anie.202214333.
- [143] Han C, Zenner J, Johnny J et al. Electrocatalytic hydrogenation of alkenes with pd/carbon nanotubes at an oil–water interface. *Nature Catalysis* 2022; 5(12): 1110–1119. DOI:10.1038/s41929-022-00882-4.

4 Research Program

- [144] Tuci G, Pilaski M, Ba H et al. Unraveling surface basicity and bulk morphology relationship on covalent triazine frameworks with unique catalytic and gas adsorption properties. *Advanced Functional Materials* 2017; 27(7). DOI: 10.1002/adfm.201605672.
- [145] von der Aßen NV, Müller LJ, Steingrube A et al. Selecting co₂ sources for co₂ utilization by environmental-merit-order curves. *Environmental Science & Technology* 2016; 50(3): 1093–1101. DOI:10.1021/acs.est.5b03474.
- [146] Postweiler P, Engelpracht M, Rezo D et al. Environmental process optimisation of an adsorption-based direct air carbon capture and storage system. *Energy & Environmental Science* 2024; DOI:10.1039/D3EE02970K.
- [147] Selmert V, Kretzschmar A, Weinrich H et al. Co₂/n₂ separation on highly selective carbon nanofibers investigated by dynamic gas adsorption. *ChemSusChem* 2022; 15(14): e202200761. DOI:10.1002/cssc.202200761.
- [148] Keller L, Ohs B, Abduly L et al. Carbon nanotube silica composite hollow fibers impregnated with polyethylenimine for co₂ capture. *Chemical Engineering Journal* 2019; 359: 476–484. DOI:10.1016/j.cej.2018.11.100.
- [149] Kipshagen A, Baums JC, Hartmann H et al. Formic acid as h₂ storage system: hydrogenation of co₂ and decomposition of formic acid by solid molecular phosphine catalysts. *Catalysis Science & Technology* 2022; 12(18): 5649–5656. DOI: 10.1039/d2cy00608a.
- [150] Mebrahtu C, Nohl M, Dittrich L et al. Integrated co-electrolysis and syngas methanation for the direct production of synthetic natural gas from co₂ and h₂ o. *ChemSusChem* 2021; 14(11): 2295–2302. DOI:10.1002/cssc.202002904.
- [151] Kabatnik C, Krekel C and Jupke A. Equilibrium studies of formic acid–amine complexation with isothermal titration calorimetry. *Industrial & Engineering Chemistry Research* 2023; 62(40): 16246–16253. DOI:10.1021/acs.iecr.3c01990.
- [152] Gausmann M, Kiefel R and Jupke A. Modeling of electrochemical ph swing extraction reveals economic potential for closed-loop bio-succinic acid production. *Chemical Engineering Research and Design* 2023; 190: 590–604. DOI: 10.1016/j.cherd.2022.12.022.
- [153] Deischer J, Müller F, Bong B et al. Separation by size exclusion: Selective liquid-phase adsorption of l-lysine from lysine–glucose mixtures on zeolites. *ACS Sustainable Chemistry & Engineering* 2022; 10(31): 10211–10222. DOI: 10.1021/acssuschemeng.2c01874.
- [154] Harhues T, Portheine L, Plath C et al. Direct electrosynthesis of 2-butanone from fermentation supernatant. *ACS Sustainable Chemistry and Engineering* 2022; 10(19): 6483–6492. DOI:10.1021/acssuschemeng.2c01971.
- [155] König A, Neidhardt L, Viell J et al. Integrated design of processes and products: Optimal renewable fuels. *Computers and Chemical Engineering* 2020; 134: 106712. DOI:10.1016/j.compchemeng.2019.106712.
- [156] Farajiamiri M, Meyer JC and Walther G. Multi-objective optimization of renewable fuel supply chains regarding cost, land use, and water use. *Applied Energy* 2023; 349. DOI:10.1016/j.apenergy.2023.121652.
- [157] Wolff M, Becker T and Walther G. Long-term design and analysis of renewable fuel supply chains – an integrated approach considering seasonal resource availability. *European Journal of Operational Research* 2023; 304(2): 745–762. DOI:10.1016/j.ejor.2022.04.001.
- [158] Walter J, Wahner F, Rudolph L et al. Method for the efficient determination of transformation paths for sector-integrated energy systems. *2023 International Conference on Future Energy Solutions, FES 2023* 2023; DOI: 10.1109/FES57669.2023.10183301.
- [159] Bongartz D, Doré L, Eichler K et al. Comparison of light-duty transportation fuels produced from renewable hydrogen and green carbon dioxide. *Applied Energy* 2018; 231: 757–767. DOI:10.1016/j.apenergy.2018.09.106.
- [160] Ebadi Torkayesh A, Hendiani S, Walther G et al. Fueling the future: Overcoming the barriers to market development of renewable fuels in germany using a novel analytical approach. *European Journal of Operational Research* 2024; DOI: 10.1016/j.ejor.2024.02.039.
- [161] Venghaus S and Hake JF. Nexus thinking in current eu policies – the interdependencies among food, energy and water resources. *Environmental Science & Policy* 2018; 90: 183–192. DOI:10.1016/j.envsci.2017.12.014.
- [162] Offermann-van Heek J, Arning K, Sternberg A et al. Assessing public acceptance of the life cycle of co₂-based fuels: Does information make the difference? *Energy Policy* 2020; 143. DOI:10.1016/j.enpol.2020.111586.
- [163] Linzenich A, Arning K and Ziefle MC. Acceptance of energy technologies in context: Comparing laypeople's risk perceptions across eight infrastructure technologies in germany. *Energy Policy* 2021; 152. DOI:10.1016/j.enpol.2020.112071.
- [164] Engelmann LV, Arning K, Linzenich A et al. Risk assessment regarding perceived toxicity and acceptance of carbon dioxide-based fuel by laypeople for its use in road traffic and aviation. *Frontiers in Energy Research* 2020; 8. DOI: 10.3389/fenrg.2020.579814.
- [165] Hendiani S and Walther G. Sustainability performance evaluation of renewable energy systems using a new multi-expert multi-criteria interval type-2 fuzzy distance to ideal solution approach. *Applied Energy* 2023; 347. DOI: 10.1016/j.apenergy.2023.121436.
- [166] Walter JD, Löhr L, Venghaus S et al. Analysis of water resources for green hydrogen production in europe. DOI: 10.18154/RWTH-2023-01580.
- [167] Borning M, Doré L, Wolff M et al. Opportunities and challenges of flexible electricity-based fuel production for the european power system. *Sustainability (Switzerland)* 2020; 12(23): 1–26. DOI:10.3390/su12239844.
- [168] Borning M, van Bracht N, Moser A et al. Electricity-based fuel production: An assessment of its impact on the european power system considering flexibility. In *2018 15th International Conference on the European Energy Market (EEM)*. IEEE. ISBN 978-1-5386-1488-4, pp. 1–5. DOI:10.1109/EEM.2018.8469916.

- [169] Grube T, Doré L, Hoffrichter A et al. An option for stranded renewables: electrolytic-hydrogen in future energy systems. *Sustainable Energy and Fuels* 2018; 2(7): 1500–1515. DOI:10.1039/C8SE00008E.
- [170] Becker T, Wolff M, Linzenich A et al. An integrated bi-objective optimization model accounting for the social acceptance of renewable fuel production networks. *European Journal of Operational Research* 2024; 315(1): 354–367. DOI: 10.1016/j.ejor.2023.11.044.
- [171] Linzenich A, Engelmann LV, Arning K et al. Harmful or beneficial to humans and the environment? an empirical study on the social acceptance and risk perception of co₂-based fuels. *Frontiers in Environmental Science* 2022; 10. DOI: 10.3389/fenvs.2022.737070.
- [172] Karbassi V, Trotter PA and Walther G. Diversifying the african energy system: Economic versus equitable allocation of renewable electricity and e-fuel production. *Applied Energy* 2023; 350. DOI:10.1016/j.apenergy.2023.121751.
- [173] Gnann T, Speth D, Seddig K et al. How to integrate real-world user behavior into models of the market diffusion of alternative fuels in passenger cars - an in-depth comparison of three models for germany. *Renewable and Sustainable Energy Reviews* 2022; 158: 112103. DOI:10.1016/j.rser.2022.112103.
- [174] Hombach LE, Büsing C and Walther G. Robust and sustainable supply chains under market uncertainties and different risk attitudes – a case study of the german biodiesel market. *European Journal of Operational Research* 2018; 269(1): 302–312. DOI:10.1016/j.ejor.2017.07.015.
- [175] Chang M, Thellufsen JZ, Zakeri B et al. Trends in tools and approaches for modelling the energy transition. *Applied Energy* 2021; 290: 116731. DOI:10.1016/j.apenergy.2021.116731.
- [176] Cuisinier E, Bourasseau C, Ruby A et al. Techno-economic planning of local energy systems through optimization models: a survey of current methods. *International Journal of Energy Research* 2021; 45(4): 4888–4931. DOI:10.1002/er.6208.
- [177] Völker S, Ackermann P, Granderath M et al. Identifying key environmental objectives for integrated process and fuel design. *Sustainable Energy and Fuels* 2024; DOI:10.1039/D3SE01602A.
- [178] Völker S, Deutz S, Burre J et al. Blend for all or pure for few? well-to-wheel life cycle assessment of blending electricity-based ome₃₋₅ with fossil diesel. *Sustainable Energy and Fuels* 2022; 6(8): 1559–1573. DOI:10.1039/d1se01758f.

PI publications not from TMFB/FSC

- [179] Schmalz F, Kopp WA, Goudeli E et al. Reaction path identification and validation from molecular dynamics simulations of hydrocarbon pyrolysis. *International Journal of Chemical Kinetics* 2024; DOI:10.1002/kin.21719.
- [180] Cai L, Jacobs S, Langer R et al. Auto-ignition of oxymethylene ethers (omen, n = 2–4) as promising synthetic e-fuels from renewable electricity: shock tube experiments and automatic mechanism generation. *Fuel* 2020; 264: 116711. DOI: 10.1016/j.fuel.2019.116711.
- [181] Choi CH, Choi WS, Kasian O et al. Unraveling the nature of sites active toward hydrogen peroxide reduction in fe–n–c catalysts. *Angewandte Chemie International Edition* 2017; 56(30): 8809–8812. DOI:10.1002/anie.201704356.
- [182] Shin D, Bhandari S, Tesch MF et al. Reduced formation of peroxide and radical species stabilises iron-based hybrid catalysts in polymer electrolyte membrane fuel cells. *Journal of Energy Chemistry* 2022; 65: 433–438. DOI: 10.1016/j.jechem.2021.05.047.
- [183] Schuppert AK, Topalov AA, Savan A et al. Composition-dependent oxygen reduction activity and stability of pt–cu thin films. *ChemElectroChem* 2014; 1(2): 358–361. DOI:10.1002/celc.201300078.
- [184] Schatz M, Jovanovic S, Eichel RA et al. Quantifying local ph changes in carbonate electrolyte during copper-catalysed co₂ electroreduction using in operando ¹³c nmr. *Scientific Reports* 2022; 12(1): 8274. DOI:10.1038/s41598-022-12264-8.
- [185] Dzięcioł K, Durmus YE, Tempel H et al. Laboratory x-ray computed tomography imaging protocol allowing the operando investigation of electrode material evolution in various environments. *iScience* 2023; 26(7): 107097. DOI: 10.1016/j.isci.2023.107097.
- [186] MacArthur KE, Polani S, Klingenhof M et al. Post-synthesis heat treatment of doped pt_{ni}-alloy fuel-cell catalyst nanoparticles studied by in-situ electron microscopy. *ACS Applied Energy Materials* 2023; 6(11): 5959–5967. DOI: 10.1021/acsaem.3c00405.
- [187] Haskins JB, Pham HH, Khetan A et al. Lithium peroxide growth in li–o₂ batteries via chemical disproportionation and electrochemical mechanisms: A potential-dependent ab initio study with implicit solvation. *The Journal of Physical Chemistry C* 2021; 125(1): 436–445. DOI:10.1021/acs.jpcc.0c08610.
- [188] Kwak D, Khetan A, Noh S et al. First principles study of morphology, doping level, and water solvation effects on the catalytic mechanism of nitrogen-doped graphene in the oxygen reduction reaction. *ChemCatChem* 2014; 6(9): 2662–2670. DOI: 10.1002/cctc.201402248.
- [189] Yildirim MH, Schwarz A, Stamatialis DF et al. Impregnated membranes for direct methanol fuel cells at high methanol concentrations. *Journal of Membrane Science* 2009; 328(1-2): 127–133. DOI:10.1016/j.memsci.2008.11.051.
- [190] Merle G, Hosseiny SS, Wessling M et al. New cross-linked pva based polymer electrolyte membranes for alkaline fuel cells. *Journal of Membrane Science* 2012; 409-410: 191–199. DOI:10.1016/j.memsci.2012.03.056.
- [191] Lauterbach L and Lenz O. Catalytic production of hydrogen peroxide and water by oxygen-tolerant nife-hydrogenase during h₂ cycling in the presence of o₂. *Journal of the American Chemical Society* 2013; 135(47): 17897–17905. DOI: 10.1021/ja408420d.

4 Research Program

- [192] Zill D, Lettau E, Lorent C et al. Crucial role of the chaperonin groes/el for heterologous production of the soluble methane monooxygenase from methylomonas methanica mc09. *ChemBioChem* 2022; 23(12): e202200195. DOI: 10.1002/cbic.202200195.
- [193] Schüth F, Palkovits R, Schlögl R et al. Ammonia as a possible element in an energy infrastructure: catalysts for ammonia decomposition. *Energy & Environmental Science* 2012; 5(4): 6278–6289. DOI:10.1039/C2EE02865D.
- [194] Schley L, Vibhu V, Nohl L et al. A highly stable pr₂nio₄+δ oxygen electrode in electrolyte supported protonic ceramic electrolysis cells (pcecs) for hydrogen production with high faradaic efficiency. *Energy Advances* 2024; 3(4): 861–873. DOI:10.1039/D3YA00542A.
- [195] Vibhu V, Vinke IC, Zaravelis F et al. Performance and degradation of electrolyte-supported single cell composed of mo-
au-ni/gdc fuel electrode and lscf oxygen electrode during high temperature steam electrolysis. *Energies* 2022; 15. DOI: 10.3390/en15082726.
- [196] Thiele P, Yang Y, Dirkes S et al. Realistic accelerated stress tests for pem fuel cells: Test procedure development based on standardized automotive driving cycles. *International Journal of Hydrogen Energy* 2024; 52: 1065–1080. DOI: 10.1016/j.ijhydene.2023.08.292.
- [197] Liu Y, Dirkes S, Kohn M et al. A high-fidelity real-time capable dynamic discretized model of proton exchange membrane fuel cells for the development of control strategies. *Journal of Power Sources* 2022; 537: 231394. DOI: 10.1016/j.jpowsour.2022.231394.
- [198] Kohn M, Liu Y, Wick M et al. A scalable pem fuel cell model for coupled mechanical and electrochemical analysis based on an analytical approach. *International Journal of Hydrogen Energy* 2024; 51: 1539–1559. DOI: 10.1016/j.ijhydene.2023.08.165.
- [199] Schmitz M and Pischinger S. Dynamic bolt forces during cold starts and drying processes of a pem fuel cell. *Journal of Power Sources* 2023; 587: 233610. DOI:10.1016/j.jpowsour.2023.233610.
- [200] Kumar A, Vibhu V, Bassat JM et al. Ammonia as a potential energy vector in the burgeoning hydrogen economy. *Chem-ElectroChem* 2024; DOI:10.1002/celec.202300845.
- [201] Mechler AK, Sahraie NR, Armel V et al. Stabilization of iron-based fuel cell catalysts by non-catalytic platinum. *Journal of The Electrochemical Society* 2018; 165(13): F1084–F1091. DOI:10.1149/2.0721813jes.
- [202] Fu Y, Ding W, Lei H et al. Spatial distribution of brønsted acid sites determines the mobility of reactive cu ions in the cu_{ssz}-13 catalyst during the selective catalytic reduction of nox with nh₃. *Journal of the American Chemical Society* 2024; 146(16): 11141–11151. DOI:10.1021/jacs.3c13725.
- [203] Rauch D, Dietrich M, Simons T et al. Microwave cavity perturbation studies on h-form and cu ion-exchanged scr catalyst materials: Correlation of ammonia storage and dielectric properties. *Topics in Catalysis* 2017; 60(3-5): 243–249. DOI: 10.1007/s11244-016-0605-z.
- [204] Kampwerth J, Weber B, Rußkamp J et al. Towards a holistic solvent screening: On the importance of fluid dynamics in a rate-based extraction model. *Chemical Engineering Science* 2020; 227. DOI:10.1016/j.ces.2020.115905.
- [205] Roth DM, Dunkel P, Kampwerth J et al. Beyond partition coefficients: Model-based solvent screening in extractive-reaction processes considering fluid dynamics and mass transfer limitations. *Industrial & Engineering Chemistry Research* 2022; 61(39): 14546–14560. DOI:10.1021/acs.iecr.2c01820.
- [206] Holzhäuser FJ, Artz J, Palkovits S et al. Electrocatalytic upgrading of itaconic acid to methylsuccinic acid using fermentation broth as a substrate solution. *Green Chemistry* 2017; 19(10): 2390–2397. DOI:10.1039/C6GC03153F.
- [207] Meyers J, Mensah JB, Holzhäuser FJ et al. Electrochemical conversion of a bio-derivable hydroxy acid to a drop-in oxygenate diesel fuel. *Energy & Environmental Science* 2019; 12(8): 2406–2411. DOI:10.1039/C9EE01485C.
- [208] Mürtz SD, Kurig N, Holzhäuser FJ et al. Reviving electrocatalytic reductive amination: A sustainable route from biogenic levulinic acid to 1,5-dimethyl-2-pyrrolidone. *Green Chemistry* 2021; 23(21): 8428–8433. DOI:10.1039/d1gc02513a.
- [209] Ren J, Zeng F, Mebrahtu C et al. Understanding promotional effects of trace oxygen in co₂ methanation over ni/zro₂ catalysts. *Journal of Catalysis* 2022; 405: 385–390. DOI:10.1016/j.jcat.2021.12.017.
- [210] Strohmam M, Vorholt AJ and Leitner W. Branched tertiary amines from aldehydes and α-olefins by combined multiphase tandem reactions. *Chemistry – A European Journal* 2022; 28(58): e202202081. DOI:10.1002/chem.202202081.
- [211] Limper A, Harhues T, Keller RG et al. Two-level porosity electrodes from metal-polymer dispersions. *Electrochemistry Communications* 2022; 135. DOI:10.1016/j.elecom.2022.107205.
- [212] Biswas S and Bolm C. Rhodium(ii)-catalyzed n-h insertions of carbenes under mechanochemical conditions. *Organic Letters* 2024; 26(7): 1511–1516. DOI:10.1021/acs.orglett.4c00216.
- [213] Pan S, Mulks FF, Wu P et al. Mechanochemical iron-catalyzed nitrene transfer reactions: Direct synthesis of n-acyl sulfonimidamides from sulfenamides and dioxazolones. *Angewandte Chemie* 2024; 136(5). DOI:10.1002/ange.202316702.
- [214] Kreissl H, Jin J, Lin SH et al. Commercial cu₂cr₂o₅ decorated with iron carbide nanoparticles as a multifunctional catalyst for magnetically induced continuous-flow hydrogenation of aromatic ketones. *Angewandte Chemie (International ed in English)* 2021; 60(51): 26639–26646. DOI:10.1002/anie.202107916.
- [215] Lin SH, Hetaba W, Chaudret B et al. Copper-decorated iron carbide nanoparticles heated by magnetic induction as adaptive multifunctional catalysts for the selective hydrodeoxygenation of aldehydes. *Advanced Energy Materials* 2022; 12(42). DOI: 10.1002/aenm.202201783.

- [216] Wang Y, Bornemann L, Reinert C et al. A method to bridge energy and process system optimization: Identifying the feasible operating space for a methanation process in power-to-gas energy systems. *Computers & Chemical Engineering* 2024; 182: 108582. DOI:10.1016/j.compchemeng.2023.108582.
- [217] Brée LC, Wessling M and Mitsos A. Modular modeling of electrochemical reactors: Comparison of co₂-electrolyzers. *Computers and Chemical Engineering* 2020; 139: 106890. DOI:10.1016/j.compchemeng.2020.106890.
- [218] Schäfer P, Schweidtmann AM and Mitsos A. Nonlinear scheduling with time-variable electricity prices using sensitivity-based truncations of wavelet transforms. *AIChE Journal* 2020; 66(10). DOI:10.1002/aic.16986.
- [219] Schweidtmann AM, Bongartz D, Grothe D et al. Deterministic global optimization with gaussian processes embedded. *Mathematical Programming Computation* 2021; 13(3): 553–581. DOI:10.1007/s12532-021-00204-y.
- [220] Hombach LE, Cambero C, Sowlati T et al. Optimal design of supply chains for second generation biofuels incorporating european biofuel regulations. *Journal of Cleaner Production* 2016; 133: 565–575. DOI:10.1016/j.jclepro.2016.05.107.
- [221] Wyndorps J, Ostovari H and von der Aßen NV. Is electrochemical co₂ reduction the future technology for power-to-chemicals? an environmental comparison with h₂-based pathways. *Sustainable Energy & Fuels* 2021; 5(22): 5748–5761. DOI:10.1039/D1SE00975C.
- [222] Löffelholz M, Weidner J, Hartmann J et al. Optimized scalable cub catalyst with promising carbon footprint for the electrochemical co₂ reduction to ethylene. *Sustainable Chemistry for Climate Action* 2023; 3: 100035. DOI: 10.1016/j.scca.2023.100035.
- [223] Nilges B, Burghardt C, Roh K et al. Comparative life cycle assessment of industrial demand-side management via operational optimization. *Computers and Chemical Engineering* 2023; 177: 108323. DOI:10.1016/j.compchemeng.2023.108323.
- [224] Nilges B, Reinert C and von der Aßen NV. Is demand-side management environmentally beneficial? analyzing the greenhouse gas emissions due to load shifting in electric power systems. *Journal of Cleaner Production* 2024; 434: 140062. DOI:10.1016/j.jclepro.2023.140062.
- [225] Germscheid SH, Nilges B, von der Aßen NV et al. Optimal design of a local renewable electricity supply system for power-intensive production processes with demand response. *Computers and Chemical Engineering* 2024; 185: 108656. DOI: 10.1016/j.compchemeng.2024.108656.
- [226] Diepers T, Müller A, Jakobs A et al. Dynamic-prospective life cycle assessment using time-explicit life cycle inventory: Methodology and implementation. In SETAC Europe Annual Meeting (ed.) *SETAC Europe 34th Annual Meeting*.
- [227] Hagedorn W, Gramlich A, Greiff K et al. Alloy and process design of forging steels for better environmental performance. *Sustainable Materials and Technologies* 2022; 34: e00509. DOI:10.1016/j.susmat.2022.e00509.
- [228] Hagedorn W, Greiff K and Pauliuk S. An environmental assessment framework for circular steel products. *Sustainable Production and Consumption* 2024; DOI:10.1016/j.spc.2024.05.031.
- [229] Bayram B and Greiff K. Life cycle assessment on construction and demolition waste recycling: a systematic review analyzing three important quality aspects. *The International Journal of Life Cycle Assessment* 2023; 28(8): 967–989. DOI: 10.1007/s11367-023-02145-1.
- [230] Hartmann JM, Shu DY, Blodau L et al. Combining life cycle assessment and planetary boundaries for sustainable energy system designs. In SETAC Europe Annual Meeting (ed.) *SETAC Europe 34th Annual Meeting*.

External publications

- [231] Galimova T, Ram M, Bogdanov D et al. Global trading of renewable electricity-based fuels and chemicals to enhance the energy transition across all sectors towards sustainability. *Renewable and Sustainable Energy Reviews* 2023; 183: 113420. DOI:10.1016/j.rser.2023.113420.
- [232] Ueckerdt F and Odenweller A. E-fuels - aktueller stand und projektionen.
- [233] statista. Distribution of oil demand in the oecd in 2022, by sector, 2024.
- [234] Senecal PK and Leach F. Diversity in transportation: Why a mix of propulsion technologies is the way forward for the future fleet. *Results in Engineering* 2019; 4: 100060. DOI:10.1016/j.rineng.2019.100060.
- [235] Dewyer AL, Argüelles AJ and Zimmerman PM. Methods for exploring reaction space in molecular systems. *WIREs Computational Molecular Science* 2018; 8(2). DOI:10.1002/wcms.1354.
- [236] Simm GN, Vaucher AC and Reiher M. Exploration of reaction pathways and chemical transformation networks. *The Journal of Physical Chemistry A* 2019; 123(2): 385–399. DOI:10.1021/acs.jpca.8b10007.
- [237] Miller JA, Sivaramakrishnan R, Tao Y et al. Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. *Progress in Energy and Combustion Science* 2021; 83: 100886. DOI: 10.1016/j.pecs.2020.100886.
- [238] Liu M, Grinberg Dana A, Johnson MS et al. Reaction mechanism generator v3.0: Advances in automatic mechanism generation. *Journal of Chemical Information and Modeling* 2021; 61(6): 2686–2696. DOI:10.1021/acs.jcim.0c01480.
- [239] Schwaller P, Probst D, Vaucher AC et al. Mapping the space of chemical reactions using attention-based neural networks. *Nature Machine Intelligence* 2021; 3(2): 144–152. DOI:10.1038/s42256-020-00284-w.
- [240] Zhang XC, Wu CK, Yang ZJ et al. Mg-bert: leveraging unsupervised atomic representation learning for molecular property prediction. *Briefings in bioinformatics* 2021; 22(6). DOI:10.1093/bib/bbab152.

4 Research Program

- [241] Rackauckas C, Ma Y, Martensen J et al. Universal differential equations for scientific machine learning. DOI: 10.48550/arXiv.2001.04385.
- [242] Owoyele O and Pal P. Chemnode: A neural ordinary differential equations framework for efficient chemical kinetic solvers. *Energy and AI* 2022; 7: 100118. DOI:10.1016/j.egyai.2021.100118.
- [243] Fjodorow P, Allmendinger P, Horvath R et al. Monitoring formaldehyde in a shock tube with a fast dual-comb spectrometer operating in the spectral range of 1740–1790 cm⁻¹. *Applied Physics B* 2020; 126(12): 1–11. DOI: 10.1007/s00340-020-07545-x.
- [244] Peters N, Krishna Pothuraju Subramanyam S, Bunce M et al. Optimization of lambda across the engine map for the purpose of maximizing thermal efficiency of a jet ignition engine. *SAE International Journal of Advances and Current Practices in Mobility* 2020; 2(6): 3140–3150. DOI:10.4271/2020-01-0278.
- [245] Hansen CM. *Hansen solubility parameters: A user's handbook*. 2nd ed. Boca Raton: CRC Press, 2007. ISBN 9780849372483.
- [246] Shaari N, Kamarudin SK, Bahru R et al. Progress and challenges: Review for direct liquid fuel cell. *International Journal of Energy Research* 2021; 45(5): 6644–6688. DOI:10.1002/er.6353.
- [247] Mansor M, Timmiati SN, Lim KL et al. Recent progress of anode catalysts and their support materials for methanol electrooxidation reaction. *International Journal of Hydrogen Energy* 2019; 44(29): 14744–14769. DOI: 10.1016/j.ijhydene.2019.04.100.
- [248] Tran K, Nguyen TQ, Bartram AM et al. A fuel-flexible alkaline direct liquid fuel cell. *Fuel Cells* 2014; 14(6): 834–841. DOI:10.1002/uce.201300291.
- [249] Gebremedhin Gebru M, Shyam Yadav R, Teller H et al. Harnessing dimethyl ether and methyl formate fuels for direct electrochemical energy conversion. *Journal of Energy Chemistry* 2023; 83: 454–464. DOI:10.1016/j.jechem.2023.05.001.
- [250] Fadzillah DM, Kamarudin SK, Zainoodin MA et al. Critical challenges in the system development of direct alcohol fuel cells as portable power supplies: An overview. *International Journal of Hydrogen Energy* 2019; 44(5): 3031–3054. DOI: 10.1016/j.ijhydene.2018.11.089.
- [251] Singh M, Zappa D and Comini E. Solid oxide fuel cell: Decade of progress, future perspectives and challenges. *International Journal of Hydrogen Energy* 2021; 46(54): 27643–27674. DOI:10.1016/j.ijhydene.2021.06.020.
- [252] Fang Q, Blum L and Stolten D. Electrochemical performance and degradation analysis of an sofc short stack following operation of more than 100,000 hours. *Journal of The Electrochemical Society* 2019; 166(16): F1320–F1325. DOI: 10.1149/2.0751916jes.
- [253] Mogensen MB, Chen M, Frandsen HL et al. Reversible solid-oxide cells for clean and sustainable energy. *Clean Energy* 2019; 3(3): 175–201. DOI:10.1093/ce/zkz023.
- [254] Deng YW, Ro SY and Rosenzweig AC. Structure and function of the lanthanide-dependent methanol dehydrogenase xoxf from the methanotroph methylomicrobium buryatense 5gb1c. *Journal of biological inorganic chemistry : JBIC : a publication of the Society of Biological Inorganic Chemistry* 2018; 23(7): 1037–1047. DOI:10.1007/s00775-018-1604-2.
- [255] Kalimuthu P, Daumann LJ, Pol A et al. Electrocatalysis of a europium-dependent bacterial methanol dehydrogenase with its physiological electron-acceptor cytochrome cjg. *Chemistry (Weinheim an der Bergstrasse, Germany)* 2019; 25(37): 8760–8768. DOI:10.1002/chem.201900525.
- [256] Lisdat F. Pqq-gdh - structure, function and application in bioelectrochemistry. *Bioelectrochemistry (Amsterdam, Netherlands)* 2020; 134: 107496. DOI:10.1016/j.bioelechem.2020.107496.
- [257] Kobayashi H, Hayakawa A, Somarathne KKA et al. Science and technology of ammonia combustion. *Proc Combust Inst* 2019; 37(1): 109–133. DOI:10.1016/j.proci.2018.09.029.
- [258] Müller M, Pfeifer M, Holtz D et al. Comparison of green ammonia and green hydrogen pathways in terms of energy efficiency. *Fuel* 2024; 357: 129843. DOI:10.1016/j.fuel.2023.129843.
- [259] Mercier A, Mounaïm-Rousselle C, Brequigny P et al. Improvement of si engine combustion with ammonia as fuel: Effect of ammonia dissociation prior to combustion. *Fuel Communications* 2022; 11: 100058. DOI:10.1016/j.jfueco.2022.100058.
- [260] Zhou L, Zhong L, Liu Z et al. Toward highly-efficient combustion of ammonia–hydrogen engine: Prechamber turbulent jet ignition. *Fuel* 2023; 352: 129009. DOI:10.1016/j.fuel.2023.129009.
- [261] Simons EL, Cairns EJ and Surd DJ. The performance of direct ammonia fuel cells. *Journal of The Electrochemical Society* 1969; 116(5): 556. DOI:10.1149/1.2411961.
- [262] Farr RD and Vayenas CG. Ammonia high temperature solid electrolyte fuel cell. *Journal of The Electrochemical Society* 1980; 127: 1478. DOI:10.1149/1.2129934.
- [263] Fournier G, Cumming IW and Hellgardt K. High performance direct ammonia solid oxide fuel cell. *Journal of Power Sources* 2006; 162(1): 198–206. DOI:10.1016/j.jpowsour.2006.06.047.
- [264] Duan C, Kee R, Zhu H et al. Highly efficient reversible protonic ceramic electrochemical cells for power generation and fuel production. *Nature Energy* 2019; 4: 230–240.
- [265] Miyazaki K, Muroyama H, Matsui T et al. Impact of the ammonia decomposition reaction over an anode on direct ammonia-fueled protonic ceramic fuel cells. *Sustainable Energy & Fuels* 2020; 4: 5238–5246.
- [266] Fabbri E, Bi L, Pergolesi D et al. Towards the next generation of solid oxide fuel cells operating below 600 °c with chemically stable proton-conducting electrolytes. *Advanced Materials* 2012; 24(2): 195–208. DOI:10.1002/adma.201103102.

- [267] Zhao Y, Setzler BP, Wang J et al. An efficient direct ammonia fuel cell for affordable carbon-neutral transportation. *Joule* 2019; 3(10): 2472–2484. DOI:10.1016/j.joule.2019.07.005.
- [268] Hu Z, Lu S, Tang F et al. High-performance precious metal-free direct ammonia fuel cells endowed by co-doped ni₄cu₁ anode catalysts. *Applied Catalysis B: Environmental* 2023; 334: 122856. DOI:10.1016/j.apcatb.2023.122856.
- [269] Almomani F and Ali H Salah Saad M. Electrochemical oxidation of ammonia (nh₄⁺/nh₃) on synthesized nickel-cobalt oxide catalyst. *International Journal of Hydrogen Energy* 2021; 46(6): 4678–4690. DOI:10.1016/j.ijhydene.2020.03.094.
- [270] Park YK and Kim BS. Catalytic removal of nitrogen oxides (no, no₂, n₂o) from ammonia-fueled combustion exhaust: A review of applicable technologies. *Chemical Engineering Journal* 2023; 461: 141958. DOI:10.1016/j.cej.2023.141958.
- [271] Grzybek G, Gryboś J, Indyka P et al. Evaluation of the inhibiting effect of h₂o, o₂, and no on the performance of laboratory and pilot k-zn_xco_{3-x}o₄ catalysts supported on α-al₂o₃ for low-temperature n₂o decomposition. *Applied Catalysis B: Environmental* 2021; 297: 120435. DOI:10.1016/j.apcatb.2021.120435.
- [272] Pochet M, Jeanmart H and Contino F. A 22:1 compression ratio ammonia-hydrogen hcci engine: Combustion, load, and emission performances. *Frontiers in Mechanical Engineering* 2020; 6. DOI:10.3389/fmech.2020.00043.
- [273] Chen S, Jelic J, Rein D et al. Highly loaded bimetallic iron-cobalt catalysts for hydrogen release from ammonia. *Nature Communications* 2024; 15(1): 871.
- [274] Urata S, Hijjiya H, Niwano K et al. Theoretical estimation of dielectric loss of oxide glasses using nonequilibrium molecular dynamics simulations. *Journal of the American Ceramic Society* 2022; 105(6): 4200–4207.
- [275] Cohen M and Vlachos DG. Modified energy span analysis of catalytic parallel pathways and selectivity. *Industrial & Engineering Chemistry Research* 2023; 62(5): 2191–2201. DOI:10.1021/acs.iecr.2c01991.
- [276] Pantelides CC, Pereira FE, Stanger PJ et al. Process operations: from models and data to digital applications. *Computers and Chemical Engineering* 2024; 180: 108463. DOI:10.1016/j.compchemeng.2023.108463.
- [277] van der Valk H, Haße H, Möller F et al. Archetypes of digital twins. *Business & Information Systems Engineering* 2022; 64(3): 375–391. DOI:10.1007/s12599-021-00727-7.
- [278] Hielscher MM, Dörr M, Schneider J et al. Labs: Laboratory automation and batch scheduling - a modular open source python program for the control of automated electrochemical synthesis with a web interface. *Chemistry, an Asian journal* 2023; 18(14): e202300380. DOI:10.1002/asia.202300380.
- [279] Mast F, Hielscher MM, Wirtanen T et al. Choice of the right supporting electrolyte in electrochemical reductions: A principal component analysis. *Journal of the American Chemical Society* 2024; 146(22): 15119–15129. DOI:10.1021/jacs.4c00910.
- [280] Dörr M, Hielscher MM, Proppe J et al. Electrosynthetic screening and modern optimization strategies for electrosynthesis of highly value-added products. *ChemElectroChem* 2021; 8(14): 2621–2629. DOI:10.1002/celec.202100318.
- [281] Breiner M, Zirbes M and Waldvogel SR. Comprehensive valorisation of technically relevant organosolv lignins via anodic oxidation. *Green Chemistry* 2021; 23(17): 6449–6455. DOI:10.1039/d1gc01995c.
- [282] Dong X, Roeckl JL, Waldvogel SR et al. Merging shuttle reactions and paired electrolysis for reversible vicinal dihalogenations. *Science (New York, NY)* 2021; 371(6528): 507–514. DOI:10.1126/science.abf2974.
- [283] Zirbes M, Graßl T, Neuber R et al. Peroxodicarbonate as a green oxidizer for the selective degradation of kraft lignin into vanillin. *Angewandte Chemie International Edition* 2023; 62(14): e202219217. DOI:10.1002/anie.202219217.
- [284] Pollok D and Waldvogel SR. Electro-organic synthesis - a 21st century technique. *Chemical science* 2020; 11(46): 12386–12400. DOI:10.1039/d0sc01848a.
- [285] Braun A, Bora DK, Lauterbach L et al. From inert gas to fertilizer, fuel and fine chemicals: N₂ reduction and fixation. *Catalysis Today* 2022; 387: 186–196. DOI:10.1016/j.cattod.2021.04.020.
- [286] Linden M, Hofmann S, Herman A et al. Electrochemical synthesis of pyrazolines and pyrazoles via 3+2 dipolar cycloaddition. *Angewandte Chemie International Edition* 2023; 62(9): e202214820. DOI:10.1002/anie.202214820.
- [287] Winter J, Prenzel T, Wirtanen T et al. Highly selective scalable electrosynthesis of 4-hydroxybenzo[e]-1,2,4-thiadiazine-1,1-dioxides. *Cell Reports Physical Science* 2024; 5(5): 101927. DOI:10.1016/j.xcrp.2024.101927.
- [288] Wiebe A, Riehl B, Lips S et al. Unexpected high robustness of electrochemical cross-coupling for a broad range of current density. *Science advances* 2017; 3(10): eaao3920. DOI:10.1126/sciadv.aao3920.
- [289] Klein M, Troglauer DL and Waldvogel SR. Dehydrogenative imination of low-valent sulfur compounds-fast and scalable synthesis of sulfilimines, sulfinamidines, and sulfinimidate esters. *JACS Au* 2023; 3(2): 575–583. DOI:10.1021/jacsau.2c00663.
- [290] Silva IdA, Bartalucci E, Bolm C et al. Opportunities and challenges in applying solid-state nmr spectroscopy in organic mechanochemistry. *Advanced materials (Deerfield Beach, Fla)* 2023; 35(52): e2304092. DOI:10.1002/adma.202304092.
- [291] Royal Society of Chemistry (ed.) *Faraday Discussions*. Royal Society of Chemistry, 2023. ISBN 978-1-83916-697-6. URL <https://pubs.rsc.org/en/journals/journalissues/fd#?issueid=fd023241&type=current&issnprint=1359-6640>.
- [292] Marvin WA, Rangarajan S and Daoutidis P. Automated generation and optimal selection of biofuel-gasoline blends and their synthesis routes. *Energy & Fuels* 2013; 27(6): 3585–3594. DOI:10.1021/ef4003318.
- [293] Restrepo-Flórez JM and Maravelias CT. Advanced fuels from ethanol – a superstructure optimization approach. *Energy & Environmental Science* 2021; 14(1): 493–506. DOI:10.1039/D0EE02447C.
- [294] Lee YS, Galindo A, Jackson G et al. Enabling the direct solution of challenging computer-aided molecular and process design problems: Chemical absorption of carbon dioxide. *Computers and Chemical Engineering* 2023; 174: 108204. DOI: 10.1016/j.compchemeng.2023.108204.

4 Research Program

- [295] Kuzhagaliyeva N, Horváth S, Williams J et al. Artificial intelligence-driven design of fuel mixtures. *Communications chemistry* 2022; 5(1): 111. DOI:10.1038/s42004-022-00722-3.
- [296] Grossmann IE, Calfa BA and Garcia-Herreros P. Evolution of concepts and models for quantifying resiliency and flexibility of chemical processes. *Computers & Chemical Engineering* 2014; 70: 22–34. DOI:10.1016/j.compchemeng.2013.12.013.
- [297] Chrisandina NJ, Vedant S, Iakovou E et al. Metrics and methods for resilience-aware design of process systems: advances and challenges. *Current Opinion in Chemical Engineering* 2024; 43: 100984. DOI:10.1016/j.coche.2023.100984.
- [298] Chang M, Thellufsen JZ, Zakeri B et al. Trends in tools and approaches for modelling the energy transition. *Applied Energy* 2021; 290: 116731. DOI:10.1016/j.apenergy.2021.116731.
- [299] Scheelhaase J, Maertens S and Grimme W. Synthetic fuels in aviation – current barriers and potential political measures. *Transportation Research Procedia* 2019; 43: 21–30. DOI:10.1016/j.trpro.2019.12.015.
- [300] Takman J and Andersson-Sköld Y. A framework for barriers, opportunities, and potential solutions for renewable energy diffusion: Exemplified by liquefied biogas for heavy trucks. *Transport Policy* 2021; 110: 150–160. DOI: 10.1016/j.tranpol.2021.05.021.
- [301] Siegrist M and Árvai J. Risk perception: Reflections on 40 years of research. *Risk analysis: an official publication of the Society for Risk Analysis* 2020; 40(S1): 2191–2206. DOI:10.1111/risa.13599.
- [302] Haywood L and Jakob M. The role of the emissions trading scheme 2 in the policy mix to decarbonize road transport in the european union. *Transport Policy* 2023; 139: 99–108. DOI:10.1016/j.tranpol.2023.06.003.
- [303] Dolge K, Barisa A, Kirsanovs V et al. The status quo of the eu transport sector: Cross-country indicator-based comparison and policy evaluation. *Applied Energy* 2023; 334: 120700. DOI:10.1016/j.apenergy.2023.120700.
- [304] Cuisinier E, Bourasseau C, Ruby A et al. Techno-economic planning of local energy systems through optimization models: a survey of current methods. *International Journal of Energy Research* 2021; 45(4): 4888–4931. DOI:10.1002/er.6208.
- [305] Baños R, Manzano-Agugliaro F, Montoya FG et al. Optimization methods applied to renewable and sustainable energy: A review. *Renewable and Sustainable Energy Reviews* 2011; 15(4): 1753–1766. DOI:10.1016/j.rser.2010.12.008.
- [306] Mancarella P. Mes (multi-energy systems): An overview of concepts and evaluation models. *Energy* 2014; 65: 1–17. DOI:10.1016/j.energy.2013.10.041.
- [307] de Meyer A, Cattrysse D, Rasinmäki J et al. Methods to optimise the design and management of biomass-for-bioenergy supply chains: A review. *Renewable and Sustainable Energy Reviews* 2014; 31: 657–670. DOI:10.1016/j.rser.2013.12.036.
- [308] Memişoğlu G and Üster H. Integrated bioenergy supply chain network planning problem. *Transportation Science* 2016; 50(1): 35–56. DOI:10.1287/trsc.2015.0598.
- [309] Li L, Manier H and Manier MA. Hydrogen supply chain network design: An optimization-oriented review. *Renewable and Sustainable Energy Reviews* 2019; 103: 342–360. DOI:10.1016/j.rser.2018.12.060.
- [310] Blanco H, Leaver J, Dodds PE et al. A taxonomy of models for investigating hydrogen energy systems. *Renewable and Sustainable Energy Reviews* 2022; 167: 112698. DOI:10.1016/j.rser.2022.112698.
- [311] Bramstoft R, Pizarro-Alonso A, Jensen IG et al. Modelling of renewable gas and renewable liquid fuels in future integrated energy systems. *Applied Energy* 2020; 268: 114869. DOI:10.1016/j.apenergy.2020.114869.
- [312] Kujanpää L, Lindroos T, Büchner D et al. Value-optimised use of biomass in a flexible energy infrastructure – summary report of era-net vabisys -project.
- [313] Axon CJ and Darton RC. Sustainability and risk – a review of energy security. *Sustainable Production and Consumption* 2021; 27: 1195–1204. DOI:10.1016/j.spc.2021.01.018.
- [314] Schweizer PJ. Systemic risks – concepts and challenges for risk governance. *Journal of Risk Research* 2021; 24(1): 78–93. DOI:10.1080/13669877.2019.1687574.
- [315] Ögmundarson Ó, Herrgård MJ, Forster J et al. Addressing environmental sustainability of biochemicals. *Nature Sustainability* 2020; 3(3): 167–174. DOI:10.1038/s41893-019-0442-8.
- [316] Svedberg P, Inostroza PA, Gustavsson M et al. Dataset on aquatic ecotoxicity predictions of 2697 chemicals, using three quantitative structure-activity relationship platforms. *Data in Brief* 2023; 51: 109719. DOI:10.1016/j.dib.2023.109719.
- [317] Gustavsson M, Käll S, Svedberg P et al. *Transformers enable accurate prediction of acute and chronic chemical toxicity in aquatic organisms*. 2023. DOI:10.1101/2023.04.17.537138.
- [318] Fantke P, Aurisano N, Bare J et al. Toward harmonizing ecotoxicity characterization in life cycle impact assessment. *Environmental Toxicology and Chemistry* 2018; 37(12): 2955–2971. DOI:10.1002/etc.4261.
- [319] Rudén C, Backhaus T, Bergman P et al. Future chemical risk management: Accounting for combination effects and assessing chemicals in groups: The report of the committee of combination of effects and assessing chemicals in groups, 2019.
- [320] Gazal AA, Jakrawatana N, Silalertruksa T et al. Water-energy-food nexus review for biofuels assessment. *International Journal of Renewable Energy Development* 2022; 11(1): 193–205. DOI:10.14710/ijred.2022.41119.
- [321] Wilkinson MD, Dumontier M, Aalbersberg IJJ et al. The fair guiding principles for scientific data management and stewardship. *Scientific data* 2016; 3: 160018. DOI:10.1038/sdata.2016.18.
- [322] Linke D, Moustakas N, Doerr M et al. nfdi4cat/voc4cat: v2024-04-08, 2024. DOI:10.5281/ZENODO.10939767.
- [323] Tremouilhac P, Lin CL, Huang PC et al. The repository chemotion: Infrastructure for sustainable research in chemistry*. *Angewandte Chemie International Edition* 2020; 59(50): 22771–22778. DOI:10.1002/anie.202007702.

5 Structures and Strategies in the Cluster of Excellence

5.1 Support of Early-career Researchers

FSC² will continue investing in the development of early-career researchers for the advancement of new research fields as well as their translation to external stakeholders and partners. Support will be provided at all early-career levels for academic, scientific and transversal skills development. Our activities will be supported by the Center for Young Academics (CYA) at RWTH, which is the overarching instrument at RWTH responsible for providing information, career development, and networking targeted towards doctoral candidates, postdocs and “Advanced Talents”. At RWTH, “Advanced Talents” denotes early-career PhD holders who are pursuing a tenured professorship. Within CYA, the RWTH Doctoral and Postdoc academies will organize a diverse range of lectures, seminars and workshops as well as coaching and advising sessions for systematic career planning, [tailored specifically for the researchers of FSC²](#). These cover training in scientific integrity, leadership, science communication, career orientation, societal translation, scientific writing and presentation skills. Such training will complement the cluster’s interdisciplinary program and impart the necessary skills for collaboration. Besides the CYA, the Center for Teaching and Learning Services (CLS) offers modular training programs, including the certificate “Professional Teaching Competences for University Teaching” to expand competence in teaching. Likewise, to promote a common leadership and supervision culture, the Center for Professional Leadership (CPL) offers certificate courses (“Leading at RWTH”), mentoring, and individual coaching. These offerings are complemented by the Family Services Center to assist with childcare and the Center for Mental Health with its confidential and free of cost psychological counselling.

5.1.1 Achievements of the early-career support measures of the FSC

The FSC’s commitment towards early-career researchers has resulted excellent outcomes at all levels. Some key examples are: (i) The FSC established or financially supported 16 professorships (Arning, von der Aßen, Backhaus, Boxx, Greiff, Herres-Pawlis, Khetan, Lauterbach, Leicht-Scholten, Magnus, Mechler, Piccini, Venghaus, Waldvogel, Wiegand, Zobel) at various levels (W1/W2/W3), including 11 new tenure-track professorships. From these, Prof. von der Aßen has been promoted from a W1 to W3 position as the director of the Chair of Technical Thermodynamics (LTT) at RWTH. Prof. Piccini has obtained a permanent position at Unimore, Modena (Italy). Prof. Rother was promoted from a W1 to a W2 position and is now being considered for a promotion to a W3 position. Prof. Khetan has completed a successful interim evaluation and is being considered for a tenured W2 position. (ii) Several postdocs of FSC, who benefited from its extensive early-career support measures, have now taken up academic positions at prestigious institutions around the globe: Jun. Prof. Delidovich (TU Wien), Jun. Prof. Becker (TU Dresden), Jun. Prof. Trotter (BU Wuppertal), Jun. Prof. Linkhorst (TU Darmstadt), Assistant Prof. Schweidtmann (TU Delft), Assist. Prof. Bongartz (KU Leuven), Prof. Wang (Beijing University of Technology), Assos. Prof. Chen (Shanghai Jiao Tong University), Prof.

Cai (Tongji University). FSC also established a JRG under the leadership of Dr. Miaomiao Du on 'Toxicity Assessment and Prediction'. (iii) FSC PhD candidate Dr. Philipp Morsch is now group leader in the FZ Jülich. Dr. Nils Kurig won the Leopoldina fellowship. (iv) The FSC Research School under the guardianship of the FSC Steering Committee, provided a systematic framework for integrating students already at the B.Sc/Bachelors level with hands-on exposure in FSC-labs on FSC-relevant research questions. Due to these measures, some of the Bachelors students were able to directly "fast track" to a PhD within the FSC. (v) The CYA provided support with 11 exclusive courses for FSC that were attended by 126 FSC participants. The topics were: Scientific Writing, Academic Presenting, Good Scientific Practice, Project Management, Scientific Poster, Time Management & Self Organization. Further, two joint seminars with three other SFBs were conducted on the topics "Nature Masterclass" and "Career Inside/Outside of Academia" to foster collaboration between the CoE and other research consortia at RWTH. (vi) The FSC financially supported over a dozen international researchers who won DAAD or similar internships. We also financially supported several incoming and outgoing researchers (B.Sc/M.Sc./PhD/Postdoc) for exchange with other universities. (vii) As a result of the scientific, structural, and financial support from FSC, two new start-ups named FXC Engineering GmbH and BioThrust were created, which are now thriving. (viii) The FSC has provided substantial support to "external" early-career researchers (all numbers from start of funding until 2023): 8 % of PhD students, 28 % postdocs from abroad, 50 % of junior professors, and 3 % of full professors were hired from abroad.

5.1.2 Early-Career Support at the FSC² Research School

Building upon the successes of the measures of the FSC, we will establish the associated FSC² Research School (FSC²RS) operated by the FSC² Steering Committee. The FSC²RS will facilitate the T-shaped growth of researchers at all levels: they specialize in contemporary and future scientific methodologies (depth) as well as comprehend systemic complexity (breadth) of a society in an energy transition phase. The broader developmental activities conducted by the CYA will be complemented by FSC²RS's cluster specific activities, e.g., lecture series, weekly seminars, colloquia with external guests (FSC² Seminar), rotational lab courses, regular retreats, seasonal schools and young researcher conferences. The FSC²RS will particularly support peer learning, exchange, and networking between their members. A mobility program with incoming and outgoing stays at internationally renowned institutes and labs will strengthen current and initiate new international cooperation networks. The measures implemented by the FSC²RS will be evaluated and further developed by an Advisory Team comprising members from the different early-career stages. The above measures will promote the ability to do research, present and publish within a challenging interdisciplinary environment, to establish a strong personal network, to gain visibility within the international community, and to ultimately make the leap into scientific independence.

5.1.2.1 Measures of Early-Career Development at the Different Stages

Undergraduate students (B.Sc./M.Sc.): FSC² will provide unique educational opportunities for undergraduates to kick-start into the cluster's research domains during their incubation phase. Besides their theses, undergraduates have the chance to partake in individual practical projects (chemistry department), team assignments (chemical and combustion engineering) as well as bursaries for the SRA-related projects (10 hours a week). Through the network of the FSC, and in particular through the International Advisory Board (IAB), undergraduates have easy access to FSC²-related industrial and international internships. Close interaction between research groups and students allows the identification and support of high potential early-career researchers. For aspiring chemists, the FSC² will establish a new Masters course of study named Sustainable Chemistry, which will be aligned with its corresponding research domains. This is a measure to identify exceptional talents and expedite their development.

Doctoral researchers: For doctoral candidates, the FSC²RS will ensure the timely formation of a dissertation committee consisting of the supervisors, which will enter into a supervision agreement with the candidate. The committee's role will be to oversee (i) content-driven team interactions within the SRAs, (ii) individual mentoring through senior and junior research group leaders, (iii) regular self-teaching activities as well as (iv) exposure and shaping of networks with outside partners and stakeholders in the form of company visits, conference participation, and visits to renowned universities. It will also design an Individualized Qualification Curriculum for their candidate consisting of both mandatory obligations and recommendations. All FSC² doctoral candidates will take part in mandatory courses on responsible research, scientific integrity, and research data management. The recommendations will be tailored to the individual needs of the candidate, and will cover topics such as Scientific Writing, Time and Self-Management, Media Competence in Teaching and Presentation, Conference English, etc. Doctoral candidates will supervise undergraduates to develop leadership skills.

Postdoctoral researchers and tenure track professors: Postdoctoral researchers will preferentially be recruited from outside to give fresh impulses and contribute additional competences. Along with the support of a mentor within the FSC², the Advanced Talents Hub in CYA will prepare postdocs for applications in highly competitive personal grant programs such as DFG Emmy Noether, EU Marie-Curie, ERC Starting Grants. It offers workshops and individual peer group and team coaching targeted towards tenure-track candidates and junior research group (JRG) leaders. Continuing the successes of FSC, FSC² will establish five new advanced postdoc-level positions as JRG leaders. These leaders will be involved in teaching and have the privilege to co-supervise at least two Ph.D. projects together with a more senior PI. Upon recommendation by the FSC² Steering Committee, and based on a rigorous evaluation procedure within the faculties, they will have the possibility to independently supervise and graduate doctoral students. Also, to offer early-career researchers promising and predictable career steps in science, RWTH offers the Junior Principal Investigator (JPI) fellowships, which are designed to attract outstanding graduates who have been abroad for at least two years. Altogether, the structural measures both from within FSC² and CYA will enhance the career prospects of post-

docs for a successful promotion to a tenured professorship. To further solidify our strengths and promote young scientists, RWTH will establish two inter-institutional professorships in coordination with MPI CEC and FZJ, see Table 6.2.1).

5.1.3 Early-Career Coordination and Funding

A Steering Committee member (von der Aßen) will be responsible for the management of the FSC²RS and its support measures for early-career researchers. The activities will be operationally supported out of the Cluster Office. These include the coordination, the conceptual design and organization of the CoE-specific curriculum in the M.Sc. and Ph.D. phase, the coordination of the scientific and the general career mentoring, coordination of internships for undergraduates, and planning of the self-teaching and lab-rotation program for Ph.D. students, CoE-specific staff development and individual career advising. He will cooperate in close synchronization with the existing early-career support structures at the CYA. The operational support of the Cluster Office is financed centrally by RWTH, see Section 6.2.

The personnel costs for JRGs "Electrocatalysts for Ammonia Fuel Cells" and "High-through-put Catalyst Synthesis and Data Driven Testing" will be covered by FSC², whereas the JRGs "AI in Reactive Fluid Dynamics", "AI/ML Data driven System analysis and Modelling" as well as all new professorships in FSC² (see Table 6.2.1) will be funded by other sources (see Section 6.2), for e.g., by applying for RWTH JPI fellowships. At FZJ, the JRG "Bio-catalytic Retrosynthesis" with a subsequent W1 appointment in the Department of Biology/Biotechnology at RWTH Aachen University is being considered. The requested instrumentation budget encompasses the start-up package for the (i) JRG "Electrocatalysts for Ammonia Fuel Cells" including an NH₃ fuel cell test station (120 k€) to investigate NH₃ DAFC applications, and (ii) for the JRG "High-through-put Catalyst Synthesis and Data Driven Testing" including a parallelized gas-phase reactor (250 k€) and online analytics (50 k€ e.g. MS, micro-GC, IR). Further project funds for all JRGs can be applied for via the Flexible Research Funds with priority (see Section 5.4.2).

Within the direct project costs (Section 4.5), travel costs for seasonal schools, international lab visits, and registration fees are included. Based on the experiences of FSC, an annual budget of 15 k€ is provided centrally by RWTH for the FSC² specific trainings, tailored and organized by CYA in close cooperation with the Cluster Office.

Table 5.1.1: Funding Request for Early-career Support

Funding category	2026	2027	2028	2029	2030	2031	2032
	Totals per year in thousand euros						
Staff	208	213	217	221	0	0	0
Total instrumentation < €150,000	120	50	0	0	0	0	0
Total instrumentation > €150,000	0	250	0	0	0	0	0
Parallelized gas-phase reactor	0	250	0	0	0	0	0

5.2 Support of Equity and Diversity

Research must address societal challenges and be socially responsible. This can only succeed in a working and research environment dedicated to the same principles. Therefore, RWTH, her partner institutions and FSC² are deeply committed to create a discrimination-sensitive, flexible and inclusive work and study environment in which everyone can thrive.

At RWTH, equity, equal opportunities and inclusion are fundamental principles of the university culture – both in studying and teaching as well as in research and in university management. These principles are based on central strategies and regulations, such as the University's Development Plan and the Inclusion Action Plan 2021-2026. At the management level, the Vice Rector for Human Resources Management and Development works closely together with the Rectorate's Staff Unit Inclusion, Gender and Diversity Management (IGaD) and the Equal Opportunities Office to monitor the implementation of RWTH's equity, diversity and inclusion policy, accompany processes and give incentives for future developments.

The university has been working on and developing its "third mission" in recent years in a participatory manner – with its Sustainability Mission Statement (2021), its Diversity Strategy 2022-2027 and its Code of Values (2024). In 2024, the project "ReaDy@RWTH", funded by HRK and BMBF, highlights the implementation of the Diversity Strategy with a broad image campaign. It underlines RWTH's claim to be an engaged university that recognizes its social responsibility and whose efforts in the area of equal opportunities extend beyond its own university boundaries. This includes e.g. supporting first generation (PhD) students and being responsible for the cross-cutting tasks of gender and diversity as part of the ENHANCE³ university alliance. RWTH's Gender and Diversity Knowledge Program will further deepen DE&I topics according to institutional interests and needs. Thus, RWTH continues to address the UN Sustainable Development Goals in their three dimensions – ecological, economic, and social.

RWTH has regularly and successfully undergone relevant certification and competition procedures in the areas of equal opportunities and family-friendliness (TOTAL E-QUALITY title since 2005; signatory of the Charta der Vielfalt since 2009, "audit family-friendly university" certificate since 2009). With a wide range of service institutions – e.g. the Family Services Center, the Center for Staff Development, the Appointments Support, the Welcome Center and the Dual Career Service, the Staff and Student Health Management – RWTH takes care of its employees and students as individuals in diverse life situations and supports them to balance work, health, and care responsibilities.

RWTH pays special attention to equal opportunities in science through university-wide measures aiming at women at all academic levels. To become more international and to further increase the number of female professors (the rise from 8 % in 2008 to 22.9 % in 2023 has already been achieved), proactive recruiting and directly addressing highly qualified candidates in Germany and abroad is a proven practice at RWTH equipped with extra funding. 20 years ago, as one of the first German universities, RWTH started the structured interdisciplinary TANDEM Mentoring Programs for female students and scientists on different levels of their career. Numerous former TANDEM participants now act as mentors for current participants.

FSC² is committed to implement and to further facilitate RWTH's vision and measures with respect to equity and diversity. In the first phase, numerous measures were taken to attract female students, doctoral and postdoctoral candidates to the cluster and promote their successful career development. Examples include special career events for women in engineering, lunch meetings with female professors as well as networking events. In order to develop tailor-made measures for the cluster, the research group Gender and Diversity in engineering (see below) develops cluster-specific measures and monitors the implementation based on actual research in gender studies in STEM. Building on the university's gender equality initiatives FSC² will cover a wide range of activities, especially in collaboration with the IGaD and the Family Services Center at RWTH: The hiring process will be continued to be overseen by the steering committee responsible for ensuring transparent and quality-driven selection of new employees. Female researchers will be encouraged to take part in RWTH's TANDEM Mentoring Programs. FSC has reached a share of 31 % of female scientists among all disciplines and hierarchies. Through its many tenure track positions, FSC has achieved 33 % female researchers on the junior-professor and professor level, including 2 of 6 coordinators of the CAs, until 2023. FSC² strives for the overall target of 30 % female researchers at all levels, especially through adapted hiring processes. To achieve these ambitious gender goals, the university will support the Cluster by talent scouting and family-friendly hiring. Moreover, FSC² intends to recruit 30 % of its PhD students internationally by advertising the positions worldwide. FSC² will prioritize ethnic diversity for tenure-track positions. To foster early intercultural awareness already at the PhD level, unconscious bias and intercultural communication trainings will be mandatory for new PhD students.

To create an inclusive research environment, FSC² will provide its employees with a supportive digital infrastructure to ensure workplace flexibility and offer easy access to childcare opportunities and lab technician support for pregnant PhD candidates and Postdocs..

In addition to the structural measures to support equity and diversity, the topic will be explored scientifically (Leicht-Scholten). Gendersensitive science and technology studies acknowledge given interdependencies between scientific, technological, and societal development. Building on existing research, the focus in FSC² will be on two areas that allow the connection of Gender Studies to the research done in the cluster to establish a conceptual basis: (i) As the cluster aims to contribute to the sustainable transformation of energy, the general relationship between gender and sustainability was researched while considering intersectional factors and how to connect these insights to engineering processes. (ii) As the cluster is researching renewable and sustainable alternatives to fossil fuels, the topic of gender identities is discussed in the context of political positions regarding environmental protection and gender equality.

Taken together, the application of this research allows the transition to an identity-relevant level (ii), which subsequently enables personal activation and thus creates an intrinsic motivation for sustainable transformation in addition to the extrinsic motivation in (i). In sum, this conceptual basis builds a transformative lens for the research conducted within the CoE that critically informs researchers about social, economic (political), and environmental factors of the design,

implementation, and use of their research. This ultimately fosters social justice and sustainable development. Furthermore, this encourages inclusivity and participation within the cluster and motivates for ethical usage of research findings for societal benefit.

Adopting this perspective enables the contribution to sustainable development on the one hand, and on the other the establishment of a point of contact in thematic proximity to the employees. As a preliminary work the organizational diversity of the cluster was assessed focusing on the factors of gender, internationality, and position, following the system-theoretical approach. Furthermore, a study design prototype was developed allowing for the research and evaluation of the event's effect. Potential results are intended to serve as a transformative impulse for the research community of the cluster as well as for gender studies or even industry.

Based on these findings, research on gender and diversity in the context of FSC² will be realized. The objective is to further explore and implement a systems-theoretical approach to diversity management within FSC² to (i) further contribute to the development of an inclusive research organization and culture, and thereby (ii) contribute to the socially responsible and sustainable development of transformative fuels. In addition to quantitative and qualitative studies, and hermeneutic efforts (i.e. analysis and interpretation of text, communication, and phenomena), practical actions that will result from the planned research have already been outlined. These include scientifically grounded workshops like for example on "Experiences of Discrimination in Scientific Research Organizations". The workshops will be accompanied by pre- and post-studies to assess the effectiveness of the measures and the level of knowledge and attitudes towards gender and diversity among cluster members. Taken together, these measures contribute to all the objectives of the FSC²: An open, inclusive and thriving research culture will be created that is receptive to novel ideas from diverse researchers, and promotes scientific excellence and innovation. Furthermore, it attracts diversity and excellence in human resource development, which, in turn, contributes to the fulfillment of all the objectives of the CoE.

5.2.1 Equity and Diversity Coordination and Funding

FSC² integrates the perspectives of gender and diversity on organizational as well as on content level, accompanied by integrated gender and diversity research (Leicht-Scholten, doctoral student). The direct costs will be used to hold workshops and provide individual support, e.g. in the form of childcare for after office hours of public childcare, training or equipment for home offices and parent-child offices at its core facilities.

Table 5.2.1: Funding Request for the Support of Equity and Diversity

Funding category	2026	2027	2028	2029	2030	2031	2032
	Totals per year in thousand euros						
Staff	67	69	70	71	73	74	76
Direct project costs (excluding staff)	10	10	10	10	10	10	10

5.3 Strategies for Research Data and Research Software Management and Provisions for Research Infrastructures and Instrumentation

As the amount of research data is rapidly growing and at the same time extremely valuable, FSC² takes various measures to make use of the research data appropriately. Building on the structures of the previous cluster and on the identified needs, the cluster aims to strengthen research data management (RDM) and enable its researchers in that regard as well as provides high-quality research infrastructure and instrumentations.

Establishing a standardized research data management (RDM) is part of RWTH's digitalization strategy. Therefore, a [central RDM team](#) offers training and consulting on RDM topics and supports the network of RDM professionals as well as [centrally provided infrastructures](#). These infrastructures include research data management organizers (RDMOs) for curating data management plans (DMPs), GitLab for code versioning, the RDM platform Coscine for handling and archiving FAIR (Findable, Accessible, Interoperable, Reusable) data [321], the electronic lab notebook eLabFTW, and the institutional repository RWTH Publications for publication of research data and software code. Financial support from the university was used to set up data steward positions in the CoEss and the university library as well as for staff in the IT Center, who supported the conceptualization and preparation of the general RDM processes at RWTH (e.g. the development of the web-based platform *Coscine*). In the upcoming phase, RWTH will supplement RDM with [new activities in the field of Research Software Engineering](#) to support the development, optimization, and maintenance of research software tools and infrastructure. A respective 'Research Software Engineering Policy' is currently being drafted to advocate for the development of FAIR software, the sharing of software code, and the enhancement of software quality. By establishing dedicated Research Software Engineering teams, the university enhances the quality and efficiency of research software development, enabling researchers to focus on scientific inquiry rather than technical implementation. This not only accelerates the pace of discovery but also promotes reproducibility and transparency in research. In addition, RWTH [reinforces the use of publicly available and open infrastructures](#) that are established in the respective scientific communities. At RWTH, a group is working to connect and further develop the Open Science practices already established in some areas. Open Access publishing is encouraged and supported by a DFG-funded publication fund and participation in the DEAL contracts.

RWTH participates in 12 NFDI consortia. Particularly relevant for FSC² are NFDI4Ing, NFDI4Cat and NFDI4Chem, in which RWTH respectively FSC² is intensively involved with its speakers (4Ing: Prof. Dr. Schmitt) or co-speakers (4Cat: Prof. Dr. Palkovits and 4Chem: Prof. Dr. Herres-Pawlis). In these consortia, tailor-made solutions for efficient data management are developed and made available to the community. These range from intensive work on international data standards for numerous methods, discipline-specific ontologies, electronic lab journals (eLNs) to discipline-specific curated repositories. NFDI4Cat has developed a controlled vocabulary [322] for digital catalysis where NFDI4Chem delivers *Chemotion* as ELN and *repo* as integrated, open-source solution for molecular data [323]. For further chemical and catalytic

data, RADAR4Chem has been established as multipurpose repository.

Further, in an international consortium, Prof. Rother is currently setting up guidelines in biocatalysis. These 'STRENDa biocatalysis guidelines' are based in standards existing for enzymology but greatly expanded to match recent and future needs in the expanding field of enzyme catalysis. For interoperability of biocatalytic data, the mark-up language *EnzymeML* was developed with participation of FSC members, which is the current tool used in the community.

The diversity of research data in engineering sciences including experimental and laboratory data, simulation data, procedures, texts, software, and complex models with thousands of parameters requires efficient data management solutions. Correspondingly, diverse approaches to managing these research data in accordance with FAIR principles were developed and applied in the FSC. While interdisciplinary collaboration in the FSC² offers a unique environment for developing innovative solutions to data management challenges, it also leads to particularly high requirements. Expert knowledge from FSC data stewards combined with the availability of suitable RDM infrastructure at RWTH Aachen University has proven key to the successful development of tailored solutions. For example, numerous detailed chemical kinetic models requiring thousands of parameters were developed within the FSC [3, 8, 9, 16, 19], [several other TMFB/FSC publications that say they are about kinetic modeling]]. The canonical representation of such data through the use of cheminformatics tools, such as the International Chemical Identifier (InChI), is well-established. In the interdisciplinary environment of the FSC, these best practices were also applied to experimental data, facilitating automatic model validation. Comprehensive curated experimental and modeling data are managed through version control tools (RWTH Aachen University *GitLab* instance), as is common practice in developing complex scientific software. Supported by RDMPs managed in RDMO, such targeted approaches lead to correct, complete, unaltered, and reliable research data that can be documented on the *Coscine* platform or through dedicated publications. In addition to the direct results achieved, the solutions developed can be applied beyond the FSC² and accelerate the development of FAIR RDM.

The FSC cluster established a [supporting structure with a data steward team](#). The team currently consists of three part-time data stewards with scientific backgrounds in the cluster's research disciplines. Therefore, they are familiar with the types of data generated in the respective fields. The data stewards support researchers by defining RDM standards, implementing the FAIR principles, and supporting in the development of tailored data management plans. With the help of data stewards and RDM training, data publications with FSC research data have been published. Moreover, with the help of JARA-Center for Simulation and Data Sciences, RWTH IT Center and the RWTH University Library, FSC has established a [RDM policy](#). This policy is in accordance with the principles of scientific data management of the participating institutions RWTH, FZJ and MPI CEC and provides guidelines for the effective handling of research data through its lifecycle. Aligning with the FAIR principles [321], the FSC policy applies to all FSC² researchers and addresses intellectual property, the use of data management plans, handling of metadata, data preservation, open access publications and deletion of

data. By signing the RDM policy, researchers feel committed to follow the policy and thereby become more aware of the topic of RDM. Teaching and training efforts for FSC² researchers will be intensified through regular RDM seminars and the highlighting of monthly “best RDM practices”. Prof. Herres-Pawlis is the spokesperson for the NFDI section Education & Training and mediates the contact for all disciplines to the RDM experts in the section.

The [introduction and use of RDMO](#) is of central importance for the cluster’s RDM strategy. RDMO offers a well-structured platform to create RDMPs by providing a framework to easily obtain information on whether and how the researcher’s data is structured and stored. These plans help organize the process of managing valuable research data, ensuring that it is efficiently collected, organized, secured and shared throughout its lifecycle. A customized catalogue is created in close cooperation with the NFDI (National Research Data Infrastructure) which allows to identify potential weaknesses and develop recommendations for future improvements of the cluster’s DMPs. The DMPs created with RDMO are assessed by the data stewards and the managing director to ensure the quality of the RDM processes.

Although FSC² and RWTH are already well equipped with RDM tools, the researchers frequently still struggle creating their DMPs and follow RDM principles. Some researchers feel overwhelmed with the creation of DMPs as it is time-consuming and choosing from the large number of tools available is difficult. These kinds of challenges are known in the RDM community and have also been observed for researchers outside the cluster. Bottlenecks of the existing structures are identified by a recently conducted extensive survey of all PhD students in the FSC, which is currently evaluated to collect information on which tools exist, are being used, and where the gaps are.

In order to complement the work of the data stewards, this cluster proposes a [concept for RDM that builds upon existing structures](#) as the cluster’s platform (see Section 5.5.1) and is [enhanced with ML](#) supportive tools. The RDM concept aims to facilitate RDM for researchers in the cluster and further develop the cluster’s platform as a single point of access (see Figure 40). As the platform is already well-known and used by the researchers, the barrier to use it for additional activities as RDM is expected to be low. The access will be designed as a research data interface that collects relevant information (metadata) about the data the researcher wants to manage. Additionally, the platform will connect to external services as RDM recommendation and guidance systems as well as RDM tools. Via this interface, researchers can get support in their decisions on which RDM tools to use and on setting up the required structures in the chosen RDM tool. Additionally, the concept aims to support the researchers in preparing data for RDM as a necessary step to ensure data quality and accessibility throughout the research lifecycle. Therefore, advanced ML models are specifically developed and implemented to assist in organizing, cleaning, and anonymizing data. These additional efforts not only enhance RDM but lowers the barrier to use the RDM tools suggested by the external guidance and recommendation service. The additional ML models tailored for the cluster’s researchers support the researchers with a state-of-the-art approach in managing the data and start RDM. In summary, data stewards will be present to answer questions regarding the RDM policy and tools and,

in addition, the proposed research data interface and the data management ML models will be available on the FSC² platform. This will ultimately support researchers in their decision-making process on RDM approaches and therefore accelerate research progress within the CoE.

Apart from the cluster's FSC platform for managing research data, RWTH provides high-quality infrastructure and services to strengthen its competitiveness and cooperation capabilities: Key infrastructures include central scientific facilities such as the IT Center, the Central Facility for Electron Microscopy (GFE), and the Central Laboratory for Micro- and Nanotechnology (ZMNT). The general openness and access to the infrastructures for a large number of scientists supports and promotes the exchange within the scientific community and the formation of national and international networks.

Together with partner institutions, RWTH has successfully established several core facilities with a lighthouse character to provide researchers with unique opportunities. These facilities meet national and international standards in terms of operation and access. In many fields, such as material development and process simulation, scientists use supercomputers to create novel insights. With JUQUEEN and JURECA, researchers in Aachen have access to a unique large-scale research infrastructure in the field of high-performance computing operated by FZJ. Both are among the most powerful supercomputers in Europe and are coordinated together with the High-Performance Computing Infrastructure "CLAIX" at RWTH. RWTH researchers also have access to the Ernst Ruska Center for Microscopy and Spectroscopy with Electrons, one of the leading infrastructures for electron microscopy in the world. It is an open user facility jointly operated by the FZJ and RWTH.

Early career researchers and junior research group leaders benefit from guaranteed access to infrastructures and core facilities during the development and pursuit of their careers. RWTH recognizes the great potential that lies in coordinating decentralized structures and bringing them into a standardized process. As such, RWTH will continue to pursue joint infrastructures that exploit the synergy potential of the university and its partners. By facilitating collaboration in interdisciplinary centers and clusters of excellence, as well as cross-faculty development, shared research infrastructures are an important asset for RWTH.

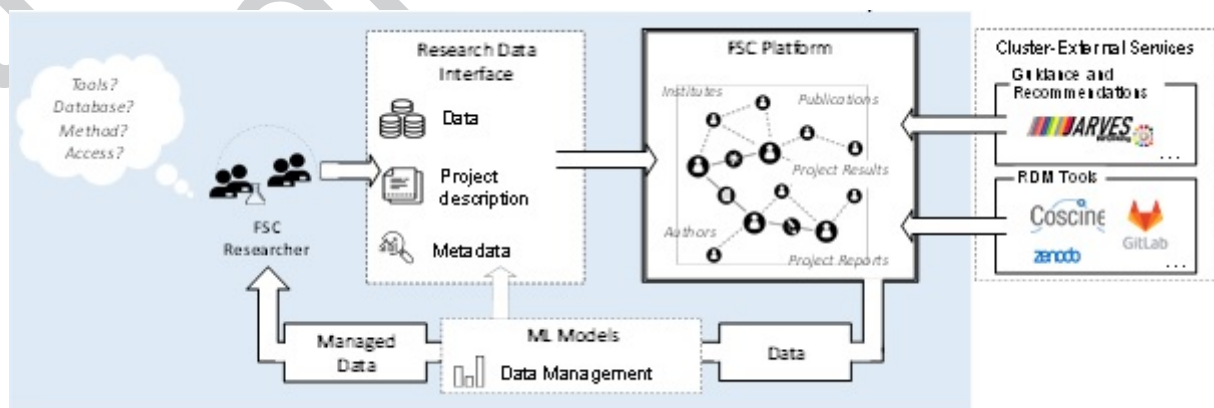


Figure 40: RDM concept within the cluster's platform.

5 Structures and Strategies in the Cluster of Excellence

5.3.1 Coordination and Funding of Research Data, Infrastructures, and Instrumentation Mgmt.

RDM measures are coordinated by the Data Steward Team under the leadership of the PI responsible for RDM (Herres-Pawlis) in close cooperation with the Cluster Office and RWTH's digitalization strategy. RWTH provides one FTE (E13-E14) for the scientists involved in the Data Steward Team. In addition, 0.5 FTE (E13), also centrally funded by RWTH, is provided for the further development and maintenance of the internal communication platform. Direct costs of 15 k€ per year include RDM software fees, IT infrastructure (especially server costs) and RDM training. All measures for the management of research data, infrastructures and instruments are financed centrally by RWTH, see Section 6.2.

5.4 Management, Governance, Quality Assurance

5.4.1 Operational Cluster Management

The CoE is a non-incorporated association of institutes of RWTH, FZJ, and the MPI CEC. All collaborations within the FSC² network are based on the jointly agreed CoE's bylaws, which describe all operational procedures. The management structure of the CoE is illustrated in Figure 41. It continues the current operational management structure of FSC that has proven to facilitate both an effective and efficient co-ordination within the cluster and the continuous development and implementation of the strategic vision of the CoE. The Operational Cluster Management consists of three pillars: the Steering Committee, the IAB, and the Cluster Office.

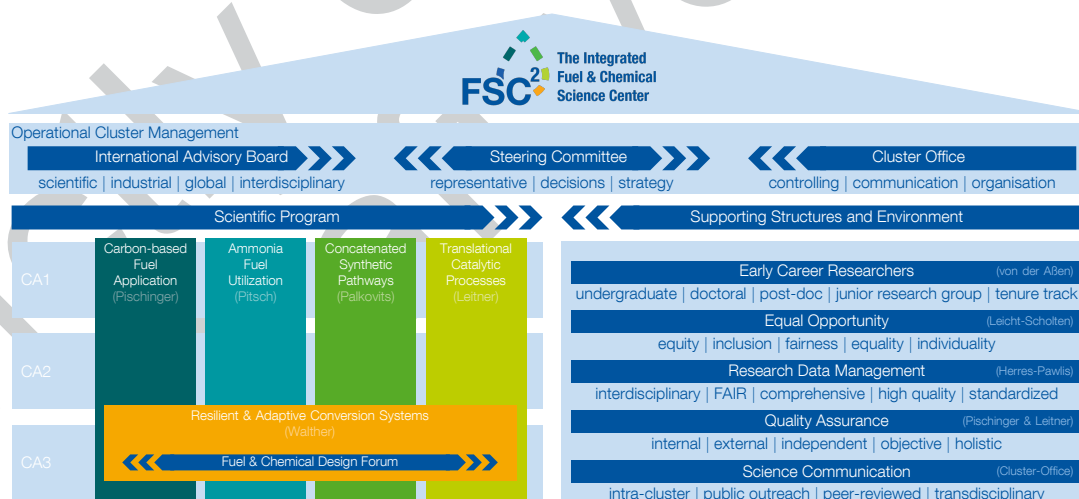


Figure 41: Management structure of the CoE

The **Steering Committee** is the central supervisory and decision-making board. The Steering Committee meets monthly. It is in charge of monitoring and steering all activities of the Scientific Program and the Supporting Structure. The Steering Committee is directed by the CoE's spokespersons Stefan Fischinger and Walter Leitner who are in charge of the scientific, technical, financial, legal, and administrative coordination. Additional members will be the coordinators of the SRAs (see Figure 41). MPI CEC and FZJ are represented by Walter Leitner and Regina Palkovits, respectively. Those responsible for the measures of the Supporting Structure

report to the Steering Committee on a monthly basis and as required. Since the spokespersons (Pischinger, Leitner) retirement will be within the next funding period, there replacements will be elected as foreseen in the CoE's bylaws.

The **International Advisory Board (IAB)** supports and monitors the CoE's activities by evaluating progress and providing impulses for further development with regard to both scientific and industrial issues. The IAB is composed of key representatives from international academic institutions and industry, related to all fields of research within FSC², insuring a close alignment of the cluster's objectives and the demands of its key stakeholders. The meeting of the IAB will take place during the annual International Conference held by FSC².

Table 5.4.1: Confirmed members of the FSC² International Advisory Board (IAB)

Name	Company/University	Position/Department
Industrial Advisors		
Dr. Jens Artz	DECHEMA	Senior Advisor E-Fuels and E-Chemicals
Dr. Marcus Bollig	VDA	Managing Director
Andreas Bulan	Covestro	R&D Manager
Prof. Dr. Maximilian Fleischer	Siemens Energy	Chief Technological Expert
Prof. Dr. Thomas Garbe	VW	Head of the Energy Carriers Subdivision
Dr. Thomas Haas	Evonik	Director Marcomolecular Chemistry
Dr. Ralf Karch	Umicore	Head of R&D Precious Metals Chemistry
Evangelos Karvounis	Ford	Director Global Powertrain R&D
Dr. Michael Krüger	Bosch	Head of Development Diesel Systems
Dr. Lars Menger	BMW AG	Specialist for Fuels and Additives
Gesa Netzeband	DGMK	Executive Director
D.Sc. (Tech) Teemu Sarjovaara	Neste Corporation	Head of R&D, Products and Applications
Dr. Peter Sauermann	BP	Director BP Global Fuels Technology
Dr. Hans-Christian Schaefer	DBU	Head of Biotechnology Division
Dr. Nicole Schödel	The Linde Group	Director of Chemical Technology Services
Dr. Marie-Noelle Semeria	TOTAL S. A.	Senior Vice President R&D One Tech
Dr. Karsten Wilbrand	Shell PLC	Senior Principal Scientist Mobility
Scientific Advisors		
Prof. Claire Adjiman	Imperial College London	Faculty of Eng., Dept. of Chemical Eng.
Prof. Paul Anastas	Yale University	Center of Green Chemistry and Eng.
Prof. Adisa Azapagic	The University of Manchester	Sustainable Industrial Systems
Prof. André Bardow	ETH Zürich	Energy and Process Systems Eng.
Prof. Alexis Bell	Energy Biosc. Institute	Chemical Eng.
Prof. André L. Boehman	University of Michigan	Dept. of Mechanical Eng.
Prof. Avelino Corma	Universidad de Valencia	Chemistry
Prof Yiguang Ju	Princeton	Dept. of Mechanical Eng., ERC
Prof. Jay Keasling	University of California	Chemical & Biomolecular Eng.
Prof. Katharina Kohse-Höinghaus	Uni Bielefeld	Dept. of Chemistry
Prof. Amit Kumar	University of Alberta	Deputy Director of Future Energy Systems
Prof. Ortwin Renn	IASS	Scientific Director
Prof. Philippe Sautet	UCLA	Catalysis, Surface Chemistry, Materials
Dr. Falco Ueckert	PIK Potsdam	Head of National Energy Transitions Team
Prof. Bert Weckhuysen	Universiteit Utrecht	Chemistry
Prof. Tao Zhang	Dalian Institute of Chemical Phsysics	Director

The **Cluster Office** consists of a Chief Operating Officer (COO) and a Chief Financial Officer (CFO) who are appointed by the coordinator of the CoE. The COO manages and supports the Steering Committee in assessing the scientific progress as well as the alignment of the individual projects to the interdisciplinary research goals of FSC². The CFO is the point of contact with the DFG financial administration. All financial management and accounting work is prepared in compliance with DFG policies. The CFO maintains financial data in relation to the activities within the CoE for all partners, and this documentation is continuously checked against the university's accounting system. As the relevance of internal and external communication as well as public outreach has increased significantly, the Cluster Office team has been expanded to include a Chief Communication Officer (CCO) (see Section 5.5). The Cluster Office is responsible for the coordination and implementation of the supporting structures. FSC researchers are supported by the measures described above, including the FSC Research School (von der Aßen, Section 5.1), Equal Opportunities (Leicht-Scholten, Section 5.2) and RDM (Herres-Pawlis, Section 5.3). Further elements of the supporting structure include **quality assurance** (Pischinger and Leitner) and **science communication** (CCO, Section 5.5).

5.4.2 Scientific Program Management and Fund Allocation

The main structural elements of the research program are the **Strategic Research Areas (SRAs)** (see Section 4.3). The SRAs have coordinators recruited from the team of PIs who coordinate and monitor the scientific progress of the individual projects. While the SRAs sustain through the period of the cluster, their project portfolio will evolve over time. Translational Research Teams (TRTs) were successfully established in the first funding period. Within the Translational Research Teams (TRTs), interdisciplinary research was carried out in temporary working groups, focusing on complex systems. The TRTs have been structurally integrated into the cluster in such a way that they function without an additional permanent organization. They continue to be supported by Flexible Research Funds, but no longer need to be embedded in the structure.

The Steering Committee decides on granting specific funding for the promotion of new research work rooted in the SRAs, as well as funding for JRGs or additional instrumentation via Flexible Research Funds. The criteria used for selecting new projects are (i) the scientific excellence of the proposed work and (ii) the relevance concerning the overall FSC² objectives. Proposals can be presented to the Steering Committee by each scientific member of the CoE. Proposals made by Early Career Researchers will be given priority. Special attention will be paid to proposals that substantially contribute to the sustainability and long-term viability of the CoE, as well as proposals that can act as a Seed Fund to attract additional third party funding.

Additional funds will be released when the newly appointed Professors start working in the CoE by shifting already started projects into the field of their responsibility and hence also adjusting the research focus. Furthermore, alignment of the projects occurs as the cluster program evolves, generating additional flexibility. A transparent and already established **internal peer project review (IPPR)** process together with a well-accepted governance will enable necessary re-adjustments and assignment of funds to new directions. Whenever project lines are discon-

tinued as part of this process, the corresponding allocated resources will be re-integrated into the Flexible Research Funds.

5.4.3 Quality Assurance

In order to ensure outstanding quality in the interdisciplinary and diverse research environment of the FSC², the established quality assurance of FSC, which already went beyond the obvious performance indicators, quality and quantity of publications, are slightly adapted. FSC² creates an environment for the researchers where the interdisciplinary work and cooperation within the cluster are especially valued by using four monitoring tools to assess the quality of individual projects and the overall research and collaboration of the cluster:

(i) Scientific progress reports on new internal communication platform in the form of interlinked [project profiles](#) (see Section 5.5), which can be continuously updated according to individual research progress, simplify both the reporting and the monitoring process. (ii) The quarterly [Fuel & Chemical Design Forum \(FCDF\)](#) supports interdisciplinary scientific exchange, identifies delays as well as potential gaps and opens up new avenues for solutions. (iii) The annual [internal peer project review \(IPPR\)](#) assesses scientific progress, cooperation within FSC², relevance for FSC², the scientific output, and, as a new indicator, the handling of research data in accordance with the FSC² RDM Policy. (iv) A combination of quantitative and qualitative evaluation methods performed by the Institute Intelligence in Quality Systems at the Laboratory for Machine Tools and Production Engineering (Isenhardt¹) inspects the inner perspective (e. g., with a [balanced scorecard evaluation](#) to quantify key indicators with respect to overall strategy, decision transparency, collaboration, education, and gender/diversity as well as [interviews with central researchers](#) within the project) as well as the outer perspective (e. g., citation count of scientific papers and references in nonscientific publications as social media or newspapers) of the scientific cooperation and work in the cluster.

5.4.4 Funding for Management, Governance, Quality Assurance

Staff for management and quality assurance comprises a Chief Operating Officer (COO), a Chief Financial Officer (CFO), a Secretary of the Cluster Office (E15-E5) and support of two student assistants (10h per week). Central Cluster Office expenses are used for e.g, software fees and IT-infrastructure at the physical Fuel Science Center, as well as set-up of technology demonstrators. Other cost include the external assessment of FSC²-developed pathways by ifeu (approx. 50 k€ per year).

Based on the experience of the current cluster, 0.5 FTEs (E13) are required for the planning, implementation, evaluation and derivation of quality assurance measures such as employee surveys (balance scorecard & interviews) and the annual internal peer project review (IPPR). All measures for management of the CoE and quality assurance will be financed centrally by RWTH, see Section 6.2.

¹Prof. Isenhardt, Associated Researcher of FSC², has already supported the CoE by developing tools to strengthen the quality assurance and the intracluster communication, e. g., the new web-based exchange platform

5.5 Science Communication, Knowledge Transfer and Research-oriented Teaching

5.5.1 Intra-cluster Communication

One of the key successes of the FSC is the thriving communication between PIs and team members across all boundaries: discipline, background, location, as well as the diversity in educational levels for the many early career scientists. Formally, intra-cluster communication will occur through coordination meetings on different levels (SRAs, Fuel & Chemical Design Forum (FCDF), general assembly, situational working groups). Intensification and documentation of intra-cluster communications are supported by RWTH-hosted software communication tools. In FSC, a comprehensive online platform was established. It is tailored to meet the diverse needs of all cluster researchers. The user-centered platform serves as a central hub for facilitating seamless communication and knowledge sharing. It encompasses a wide array of features such as (i) contact information for each researcher to facilitate easy connectivity, (ii) detailed, searchable information about every project in a project profile interlinked with the scientific output and cooperating projects, (ii) all cluster publications to enable cluster-wide literature research, and (iii) the collaborative FSC² fuel database to document and support ongoing research. As a central contact point within the cluster, this platform will be further optimized to users' needs and enriched with new features, for example to facilitate RDM within the cluster.

5.5.2 External Scientific Communication

As successfully² implemented in FSC, external scientific communication will be primarily achieved through the publication of scientific results in renowned international journals, book contributions, monographs and conference proceedings. Additionally, FSC² invites national and international scientists to participate in its own annual international conference held in Aachen: "Fuel Science: From Production to Propulsion"³. With recently over 300 participants, the conference has consistently been a resounding success. Even during the global pandemic of 2020, the conference continued in an online format. A novel hybrid format was subsequently devised to permit an even larger group of interested participants to attend the conference.

RWTH Aachen aims to generate and transfer knowledge to society through open dialogues and new instruments like the Knowledge Hub. In today's complex world, the university emphasizes the importance of distinguishing reliable information and strengthening trust in research. RWTH commits to transparent and accessible knowledge sharing, participates in social discourse, and offers innovative solutions, such as transforming former coal mining regions, while engaging with societal actors to foster respectful scientific communication.

5.5.3 Societal Communication

The newly established CCO serves both as an internal point of contact for cluster members for the publicly effective presentation of their scientific successes and for coordinating exter-

²Google Scholar Profile "The Fuel Science Center": >400 publications with >6500 citations

³from 2013 to 2018 "Tailor-Made Fuels – From Production to Propulsion"

nal requests, such as contributions to television programs and interviews (see examples in Appendix A.2). In order to maintain a constant flow of information, the CCO initiated a continuously updated science communication plan. In order to further promote the dissemination of research results in society and politics, FSC works closely with the press and communications departments of the participating institutions, the Deutsche Forschungsgemeinschaft (DFG) (e.g. contributions to the annual American Association for the Advancement of Science (AAAS)), the consortia of the Excellence Initiative (e.g. the podcast "Exzellent erklärt") and other organizations such as NRW.Energy4Climate. The society is constantly informed about the activities of the CoE on its website and the FSC Newsletter. The cluster represents itself also on exhibitions, fairs and conferences, for example in context of EuropCat (Aachen, 2019), "Tag der Neugier" (FZJ, 2019 & 2022) and "Woche der Umwelt" (digital, 2020). The cluster's social media presence has been expanded to include an Instagram, X and LinkedIn.

5.5.4 Knowledge Transfer

At RWTH, transfer is based on research adding value to the economy and society through the continuous exchange of ideas, knowledge, technologies, and people. It is a central component of RWTH's strategy, involving intellectual property valorization, industrial research cooperation, start-up support, and the involvement of creative people, shaping social change.

The greatest impact is achieved through collaboration with strategic partners and integrating new, internationally visible fields of action in transfer: (i) Scaling through collaboration with partners increases resources and impact in the IP area, e.g., for exploiting life science technologies. (ii) Quantitative increase in inventions and spin-offs comes from active scouting of research ideas, enabling better management and communication of transfer activities. (iii) New formats like the Collective Incubator, Frontier Workshops, Living Labs, and Techathons drive continuous exchange among transfer actors, coordinated by a central university contact point. (iv) Translation focuses on adapting technology for specific applications, orchestrating interactions between researchers, industry, start-ups, and society to address grand societal challenges.

This strategic efforts are supported by the work of the FSC². With its interdisciplinary scientific structure FSC² offers an ideal basis for successful knowledge transfer. Researcher of FSC have initiated respectively participated in numerous multilateral application-related research networks, like BMBF: Kopernikus, Carbon2Chem®, NamoSyn, METAFOR, Clusters4Future Hydrogen; BMWK(formerly BMWi): C³-Mobility, MethQuest, Power-to-MEDME-FuE; EU: RED-IFUEL, MIX-UP, TAKE-OFF; MWIKE: SCI4climate.NRW (2018-2022). The cluster PIs also provide assistance to its members in the establishment of new businesses. Successful start-ups with a direct link between the founders and the FSC are: (i) BioThrust GmbH, which develops a bioreactor with a patented membrane architecture for bubble-free gas exchange, providing stress-free cultivation conditions to achieve higher cell concentrations and quality, with the fastest CO₂ pH control and no need for antifoam, and (ii) FXC Engineering GmbH, who invented the concept of a flex-X-cell designed as a modular, adaptable and scalable platform cell for a wide range of electrochemical applications.

5.5.5 Research-Oriented Teaching

RWTH adopted a new teaching and learning mission statement for education in early summer 2023. In this mission statement, the university specifically addresses research-oriented teaching. With its strong focus on research in teaching, RWTH encourages and empowers its students from an early stage to engage in diverse, forward-looking fields of research and innovation.

A Blended Learning environment was established in FSC to educate early career researchers from various disciplines on different education levels. In this manner, it is possible to ensure that effective integration into the extensive research portfolio of FSC will be accomplished. The Blended Learning environment combines face-to-face teaching with digital learning. For the digital learning the platform “Moodle” is used. All teaching materials are available on this platform and are accessible for all PIs and PhD students of the CoE.

5.5.6 Coordination and Funding for Science Communication, Knowledge Transfer, and Research-Oriented Teaching

The activities in science communication, knowledge transfer, and research-oriented teaching will be coordinated centrally by the Cluster Office. Based on the experiences of the current cluster, 0.5 FTE (E11) with support of two student assistants (10h per week) is required for staff. Direct project cost include budget for the yearly held international conference and outreach activities (e.g. fairs, marketing, social media). Further, direct cost encompasses hardware (touchscreens and laptops), and display material such as roll-ups.

All measures for science communication, knowledge transfer, and teaching will be financed centrally by RWTH, see Section 6.2.

6 Environment of the Cluster of Excellence

6.1 Strategic Development Planning at the Applicant University

The vision of RWTH is to foster a unique educational and research environment that creates knowledge, transfers it to the next generation of researchers, industry and society and discovers solutions that impact current and future technical and scientific challenges. Therefore, RWTH will continue to grow beyond a unique integrated, interdisciplinary university by embracing the convergence of knowledge, approaches and insights from the humanities, economics, engineering, natural and life sciences, i.e. biology and medicine.

A common core activity of RWTH's research portfolio will be the comprehensive analysis, description, understanding and design of complex systems. Interactions of single system elements determine the dynamics of complex systems and must be understood with disciplinary depth. However, a holistic understanding of complex systems requires interdisciplinary breadth, with the integration of many competences and methodologies across disciplines as a fundamental necessity. Increasing societal and governmental demands for knowledge valorization affect the balance between curiosity-driven knowledge creation and application-driven engineering solutions. The FSC² plays a key role in this process by integrating natural, life, and engineering sciences with social and economic sciences.

RWTH embodies a broad knowledge and competence landscape that supports frontier research. In nine interdisciplinary Profile Areas, internationally recognized researchers with expertise from basic research to highly specialized applications work together to develop innovative and sustainable solutions for the future, transforming ideas into innovations. This is accomplished in collaboration with national and international partners. The Profile Areas are the breeding ground of the University. Their achievements are reflected in the current and new research networks, the ongoing CoEs as well as the activities to initiate new CoEs. The CoEs exemplify RWTH's research model and serve as a blueprint for RWTH's further development. This approach is ultimately based on the genetic code of the University, namely the ability to create knowledge and to transfer it to increase the impact of research via strong research networks. New proposals for CoEs, which have been critically reviewed by the Rectorate, faculties and the Profile Areas, are a direct result of this approach.

To foster an open research culture, to empower people at all career levels by acknowledging their different professional development needs, and to establish an agile institutional framework, governance structures and strategic partnerships, the CoEs are closely interlinked with the five strategic objectives of RWTH for the second funding line, University of Excellence (UoE):

(i) leverage RWTH's interdisciplinary research culture, (ii) develop a value-chain of knowledge from teaching to transfer (iii) nurture talents, empower people and boost teamwork, (iv) strengthen existing and building new alliances, (v) tune the agile governance culture.

6.2 Resources Provided by the Institutions

6.2.1 Staffing

The institutional personal resources of the PIs and the associated researchers ensure a highly competent critical mass with long-standing experience in the relevant research fields and methodologies. From the 25 core PIs of FSC², several hold dual appointments at RWTH and either in the Helmholtz-Association or the Max Planck Society (see Section 4.4). It is estimated that about 20 % of the staff at the participating institutes will be directly involved in the scientific program of FSC², but not financed by the CoE. This includes, in addition to the total of 37 professors, around 15 postdocs, 25 doctoral students and 50 technical/administrative staff.

The participating institutions will offer major support to the FSC by providing funding and hiring new faculty, as shown in Table 6.2.1. These faculty members will bring necessary and complementary expertise to the CoE. FSC plans to integrate more researchers as the TRTs evolve. This will create a dynamic structure with a stable core that can adapt in terms of content and expertise as needed.

Table 6.2.1: New tenure track and lighthouse appointments generated within the FSC²

Level	Topic	Sustaining Institution / Host	Model
W1/W2	Modelling & Simulation in Catalysis	RWTH, Fac. Nat. Sciences	Tenure Track
W3	Inorganic Chemistry and Electrochemistry	RWTH, Fac. Nat. Sciences	Lighthouse
W3	Sustainable Chemical Process Engineering	RWTH, Fac. Mech. Eng.	Lighthouse
W3	Fluid Mechanics	RWTH, Fac. Mech. Eng.	Lighthouse
W3	Heat and Mass Transfer	RWTH, Fac. Mech. Eng.	Lighthouse
W3	New Methods for Organic Synthesis	RWTH, Fac. Nat. Sciences	Lighthouse
W3	Techn. Acceptance, Risk Communication	RWTH, Fac. Arts & Humanities	Lighthouse
W3	Energy Conversion for Mobile Propulsion	RWTH, Fac. Mech. Eng.	Lighthouse
W3	Molecular Science and Engineering	RWTH, Fac. Nat. Sciences	Lighthouse
W2	Catalyst Development	RWTH/FZJ, Fac. Nat. Sciences	interinst.
W3	Digital Chemistry	MPG FG (CEC)/RWTH, Fac. Nat. Sciences	interinst. Lighthouse
W3	Fuel Cell Beyond H ₂ : Electro-organic Molecular Conversion	RWTH, Fac. Mech. Eng.	Lighthouse

6.2.2 Additional Funding Provided by Institutions

Next to core support for staffing and infrastructure, the participating institutions and the State of North-Rhine-Westphalia directly support the research of FSC² by funding numerous early career researchers and the corresponding measures for early career support (see Section 5.1), research data management measures (see Section 5.3), cluster management and quality assurance (see Section 5.4) as well as science communication (see Section 5.5) and external collaborations (See Section 6.3). Three new JRGs will be established and funded, two by RWTH and one by FZJ. Moreover, RWTH provides Flexible Research Funds totaling 2.55 Mio. € for the promotion of new research work and additional support of the JRGs (see Section 5.4.2). Two

W3 professorships, "Digital Chemistry" and "Fuel Cell Beyond H2: Electro-organic Molecular Conversion", will, if this proposal is successful, be permanently funded and supported in terms of personnel and equipment by the state of North Rhine-Westphalia in the amount of 450 k€ per year each. In addition, the CoE can apply for funds awarded by RWTH Aachen University to support research projects that are not yet eligible for third-party funding. In particular, the funding of JRGs via the JPI program is targeted here.

Table 6.2.1: Funding provided by the institutions

Funding category		2026	2027	2028	2029	2030	2031	2032	Total
Totals in thousand euros									
Early Career Support	Staff	104	213	325	332	362	485	259	2 185
	Other costs	15	15	15	15	15	15	15	
Research Data Management	Staff	108	111	113	115	117	120	122	910
	Other costs	15	15	15	15	15	15	15	
Management & Quality Assurance	Staff	303	309	315	322	328	335	341	2 842
	Other costs	83	83	84	84	85	85	85	
Science Communication	Staff	30	31	31	32	32	33	34	1 197
	Other costs	138	138	139	139	140	140	140	
External Collaboration	Other costs	10	10	10	10	10	10	10	70
Flexible Research Funds	Staff & instr.	250	600	600	500	200	200	200	2 550
Total funding provided		1 057	1 525	1 647	1 564	1 304	1 437	1 222	9 755

6.2.3 Infrastructural Framework

The PIs at RWTH and their partner institutions have access to state-of-the-art research facilities and instrumentation, enabling them to conduct their work at the highest level. To optimize collaboration, the activities within FSC are strategically coordinated via a virtual as well as in a physical center: the The Fuel Science Center building providing 1000 m² laboratory space and 600 m² office space also used to host international guest researchers and for teaching and educational purposes. Additionally, the FSC has access to the infrastructure of RWTH's profile areas as well as its partner institutions (FZJ & MPI CEC)

The Center for Mobile Propulsion (CMP) and the Center for Next Generation Processes and Products (NGP²) are also accessible for the FSC. The CMP pursues interdisciplinary research on electrified hybrid powertrains, which interacts with the research activities of the FSC. The NGP² deals with multi-scale process development from micro-liter to liter scale, which is also essential for the sustainable production of fuels.

The FSC also has access to the testing facilities of the Aldenhoven Testing Center, funded by the European Union (EU) and the state of North Rhine-Westphalia. At the center interdisciplinary testing for mobility is conducted.

The Competence Center on Industrial Electrochemistry (ELECTRA) was developed by the Chair of Chemical Process Engineering at RWTH (Wessling) and the IEK-9 of the FZJ (Eichel). ELECTRA deals with the acceleration of the the development of electrochemical processes.

The Institute of Technical and Macromolecular Chemistry (ITMC) has received approximately

four million euros in funding to develop an incubator infrastructure called “QuinCAT” with the goal of fostering an atmosphere conducive to entrepreneurial spirit and advancing developments in green chemistry from laboratory scale to a point where they can be commercialized. Via the Jülich Aachen Research Alliance (JARA) computing time contingents are exclusively dedicated to researchers from RWTH and FZJ. Researcher of RWTH can use up to 800 TFlops on JURECA Booster and up to 450 TFlops on CLAIX2016. 100 TFlops are reserved for RWTH researchers on JURECA. The contingents were increased to 2000 TFlops on the CLAIX2018 cluster and 250 TFlops at a Tier-3 cluster at ITC.

6.3 Collaboration with External Partners

The principal investigators of the FSC established over the years a continuously growing number of national and international collaborations of relevance for FSC. The [Aachen-California Network of Academic Exchange \(ACaINet\)](#), was a DAAD-supported network between RWTH and three campuses of the University of California (Berkeley, Los Angeles, and Santa Barbara) with the main objective of student and researcher exchange in the fields of catalysis and NMR science. A follow-up application is planned for this year. The [University of Alberta](#) has been awarded the Future Energy Systems research initiative as part of Canada’s First Research Excellence Fund competition. Due to the strong content-related and structural links, the FSC contributes significantly to strengthening the institutional partnership, e.g. through the exchange of researchers and joint courses. The FSC has established an annual exchange meeting with [e-Refinery](#) and [VoltaChem](#), which will be continued in FSC². The Federal Ministry of Education and Research (BMBF) has launched the [Kopernikus Projects for Energy Transition](#), a series of major nationwide networks involving academic and industrial partners. FSC PIs play leading roles in two of these projects, [Power-To-X](#) (Leitner, Eichel) & [SynErgie](#) (Mitsos). The [CAT Catalytic Center](#) is a long-term (10 Years) strategic collaboration between RWTH and the company Covestro, with currently about 28 young researchers and technicians. It is a successful example for translational research on catalytic CO₂ conversion in public private partnerships. To facilitate collaboration between high-level academic and industrial teams across Europe and to encourage student mobility, RWTH is a collaborating institution within the European Doctoral Program on [Sustainable Industrial Chemistry \(SINCHEM\)](#), which is hosted by the University of Bologna, Italy. [Renewable Fuels and Chemicals for Switzerland \(refuel.ch\)](#) is a project of the ETH Domain funded by the Swiss Federal Office of Energy’s SWEET program with the mayor objective to develop an interdisciplinary understanding of robust and sustainable pathways for chemicals and fuels. FSC is a Round Table-cooperation Partner of this project. Founded in 2010 by FZJ, RWTH and the universities of Düsseldorf and Bonn, the [Bioeconomy Science Centre \(BioSC\)](#) contributes to the development of a sustainable bioeconomy. Over 70 institutes and working groups are currently members of the BioSC including numerous PIs from FSC. The [Bio4MatPro](#) competence centre combines the capabilities of the research and industrial landscape in Rhenish mining area (Rheinische Revier) and in NRW for the biological transformation of materials science and production technology (von der Aßen, Blank, Jupke, Klankermayer, Palkovits). Together with stakeholders from business, agriculture, research, ed-

education, local authorities and the public, the [BioökonomieREVIER](#) initiative is pursuing the goal of developing the Rhenish mining area into a model region for sustainable economic activity with international appeal. (Jupke: deputy of the executive board, Blank, Mitsos). [AUFBRUCH](#), financed by the BMBF, is a new graduate cluster. A total of 37 PIs, 7 from FSC with their PhD students from RWTH Aachen University, FH Aachen, Forschungszentrum Jülich GmbH, HHU Düsseldorf, TH Köln, and TU Dortmund collaborate in six innovation areas on different topics to shape the transformation of the Rhenish mining area. FSC collaborates closely with the BMBF funded [Clusters4Future](#) initiatives [ETOS](#) and [Hydrogen \(H₂\)](#). The link to ETOS is through its speaker, Prof. Waldvogel, who also serves as a PI within FSC, with shared interests in electroorganic synthesis. In H₂, FSC PIs (Pischinger, Mechler, Wessling) play pivotal roles. This synergy is underpinned by the shared focus on electrochemical conversion. [HYDROGENi](#) is a Norwegian Centre for Environment-friendly Energy Research aiming to develop knowledge methodologies and innovative solutions for H₂ energy carriers (H₂ and NH₃) covering the entire value chain and including research on ammonia engines. Synergies between FSC² and HYDROGENi will be utilized with potential exchange of students and doctoral candidates. [Decarbonization of Thermal Processes in Manufacturing](#) is a large-scale project in Japan funded by NEDO at a level of up to 35 billion Yen. The research within this project on industrial burner systems will complement the work at FSC² on ammonia combustion engines. Collaborations with the projects have already started with student exchanges. The [International Research Training School Hy-Potential](#) at RWTH Aachen University and the Tokyo Institute of Technology considers different aspects along the hydrogen life-cycle including production, storage and transport, electrochemical and thermochemical conversion, and life-cycle and socio-economic assessment. Several Hy-Potential PIs are part of FSC² and will bring the complementary expertise. [KOALA](#) is an interdisciplinary cooperation platform established by the MPI CEC (Leitner) and the RWTH (Palkovits) with the objective of translating scientific knowledge and expertise into practical applications. The [SusChemSys](#) doctoral network operates at the interdisciplinary intersection of chemistry and process engineering. Its doctoral students belong to various universities and external research institutions in NRW including RWTH, the MPI CEC, and the Max Planck Institute for Coal Research and five industrial partners (ALTANA AG, Evonik Industries AG, Henkel AG & Co. KGaA, Jowat SE, OQ Chemicals GmbH). The future research center [catalaix: Catalysis for Circular Economy](#) was selected as the winner of the Werner Siemens-Foundation's ideas competition. The research team including numerous FSC PIs, led by Prof. Klankermayer and Prof. Palkovits outperformed 122 other submissions.

6.3.1 Coordination and Funding for Collaboration with External Partners

The activities in collaboration with external partners, e.g. symposia and workshops, are coordinated centrally by the Cluster Office and financed by RWTH, see Section 6.2. The direct project cost (Section 4.5) including travel cost.

7 Funding Request

Table 7.1: Total Funding Requested for the Research Program

Research Subunits	Funding Category	Total* 2026–2032
SRA “Carbon-based Fuel Application”	Staff	6 388
	Direct project costs (excl. staff)	1 431
	Instrumentation	732
SRA “Ammonia Fuel Utilization”	Staff	8 333
	Direct project costs (excl. staff)	1 535
	Instrumentation	755
SRA “Concatenated Synthetic Pathways”	Staff	11 943
	Direct project costs (excl. staff)	2 156
	Instrumentation	885
SRA “Translational Catalytic Processes”	Staff	9 166
	Direct project costs (excl. staff)	1 716
	Instrumentation	895
SRA “Resilient & Adaptive Conversion Systems”	Staff	8 333
	Direct project costs (excl. staff)	1 260
Total		55 527

* as detailed in Tables 4.5.1.4 to 4.5.5.4; amounts in thousand euros

Table 7.2: Total Funding Requested for Structural Measures

Structural Measures	Total* 2026–2032
Early-career Researchers	1 279
Equity and Diversity	570
Total	1 849

* as detailed in Tables 5.1.3 and 5.2.1; amounts in thousand euros

Table 7.3: Total Staff Requested

Staff category	2026	2027	2028	2029	2030	2031	2032
	Number of staff positions						
Independent junior research group leaders	2	2	2	2	0	0	0
Postdoctoral researchers	14	14	14	14	14	14	14
Doctoral researchers	70	70	70	70	70	70	70

Table 7.4: Total Funding Requested

Funding category	2026	2027	2028	2029	2030	2031	2032	Total
Totals in thousand euros								
Staff	6 216	6 340	6 467	6 596	6 503	6 633	6 766	45 521
Direct project costs (excl. staff)	1 479	1 559	1 139	1 009	994	994	994	8 168
Instrumentation	1 625	1 647	260	100	55	0	0	3 687
Total project funding	9 320	9 546	7 866	7 705	7 552	7 627	7 760	57 376

A Appendix

A.1 The 25 most important publications for the Cluster of Excellence, Category A

1. Ackermann, Philipp, et al. "Designed to Be Green, Economic, and Efficient: A Ketone-Ester-Alcohol-Alkane Blend for Future Spark-Ignition Engines." *ChemSusChem* 14.23 (2021): 5254-5264.
2. Aigner, Maximilian, et al. "Model-based equipment design for the biphasic production of 5-hydroxymethylfurfural in a tubular reactor." *AIChE Journal* 66.4 (2020): e16849.
3. Becker, Tristan, et al. "An integrated bi-objective optimization model accounting for the social acceptance of renewable fuel production networks." *European Journal of Operational Research* 315.1 (2024): 354-367.
4. Bordet, Alexis, et al. "Selectivity control in hydrogenation through adaptive catalysis using ruthenium nanoparticles on a CO₂-responsive support." *Nature chemistry* 13.9 (2021): 916-922.
5. Burre, Jannik, et al. "Comparing pathways for electricity-based production of dimethoxymethane as a sustainable fuel." *Energy & Environmental Science* 14.7 (2021): 3686-3699.
6. Fleitmann, Lorenz, et al. "Molecular Design of Fuels for Maximum Spark-Ignition Engine Efficiency by Combining Predictive Thermodynamics and Machine Learning." *Energy & Fuels* 37.3 (2023): 2213-2229.
7. Graf von Westarp, William, et al. "Interdisciplinary development of an overall process concept from glucose to 4, 5-dimethyl-1, 3-dioxolane via 2, 3-butanediol." *Communications chemistry* 6.1 (2023): 253.
8. Grütering, Carolin, et al. "Acetoin production by resting cells of *Lactococcus lactis* for direct electrochemical synthesis of 2-butanone." *Green Chemistry* 25.22 (2023): 9218-9225.
9. Grütering, Carolin, et al. "Methyl ketones: a comprehensive study of a novel biofuel." *Sustainable Energy & Fuels* 8.9 (2024): 2059-2072.
10. Honecker, Christian, et al. "Molecularly-controlled high swirl combustion system for ethanol/1-octanol dual fuel combustion." *Fuel* 345 (2023): 128184.
11. Hueffel, Julian A., et al. "Accelerated dinuclear palladium catalyst identification through unsupervised machine learning." *Science* 374.6571 (2021): 1134-1140.
12. Jacobs, Sascha, et al. "A comprehensive experimental and kinetic modeling study of the combustion chemistry of diethoxymethane." *Energy & Fuels* 35.19 (2021): 16086-16100.
13. Kohlhaas, Yannik, et al. "Electrochemical urea synthesis." *Joule* (2024).
14. Mendel, Marvin, et al. "Dynamic stereomutation of vinylcyclopropanes with metalloradicals." *Nature* (2024): 1-7.
15. Merchan, Angel L., et al. "Chemical recycling of bioplastics: technical opportunities to preserve chemical functionality as path towards a circular economy." *Green Chemistry* 24.24 (2022): 9428-9449.
16. Alvarez, Ariel A. Schönberger, et al. "Impact of unintentionally formed CH₂O in oxygenated fuel exhausts on DeNO_x-SCR at different NO₂/NO_x ratios under close to real conditions." *Catalysis Science & Technology* 13.14 (2023): 4069-4081.

17. Simböck, Johannes, et al. "Electronic parameters in cobalt-based perovskite-type oxides as descriptors for chemocatalytic reactions." *Nature communications* 11.1 (2020): 652.
18. Spöring, Jan-Dirk, et al. "Effective Production of Selected Dioxolanes by Sequential Bio- and Chemocatalysis Enabled by Adapted Solvent Switching." *ChemSusChem* 16.2 (2023): e202201981.
19. Bardow, André, et al. "Towards carbon-neutral and clean combustion with hydroformylated Fischer-Tropsch (HyFiT) fuels." (2023).
20. Wang, Changlong, et al. "A Novel Electrode for Value-Generating Anode Reactions in Water Electrolyzers at Industrial Current Densities." *Angewandte Chemie International Edition* 62.7 (2023): e202215804.
21. Ziegler, Anita L., et al. "Simultaneous design of fermentation and microbe." *AIChE Journal* (2024): e18501.
22. Zimmerman, Julie B., et al. "Designing for a green chemistry future." *Science* 367.6476 (2020): 397-400.
23. Meyers, Jérôme, et al. "Electrochemical conversion of a bio-derivable hydroxy acid to a drop-in oxygenate diesel fuel." *Energy & Environmental Science* 12.8 (2019): 2406-2411.
24. Bartalucci, Ettore, et al. "The effect of methyl group rotation on ^1H - ^1H solid-state NMR spin-diffusion spectra." *Physical Chemistry Chemical Physics* 25.29 (2023): 19501-19511.
25. Bartalucci, Ettore, et al. "Disentangling the Effect of Pressure and Mixing on a Mechanochemical Bromination Reaction by Solid-State NMR Spectroscopy." *Chemistry—A European Journal* 29.12 (2023): e202203466.

Guidelines for A.2:

Here you can cite any other form of published research results. Please provide a list of up to 25 other published scientific or scholarly outcomes, e.g. articles on preprint servers and non-peer reviewed contributions to conferences or anthology volumes, recensions/reviews without peer review, data sets, protocols of clinical trials, software packages, patents applied for and granted, blog contributions, infrastructures or transfer. You may also indicate other forms of scientific or scholarly output such as contributions to the (technical) infrastructure of an academic community (including in an international context) or contributions to science communication.

Estimation:

A.2 The 25 most important publications for the Cluster of Excellence, Category B

Strictly confidential
draft version

Guidelines for A.3:

Please list up to 25 additional important indicators (not including publications) which, in your view, highlight the qualifications of the principal investigators (research awards, third party funding, etc.). You may also briefly note the relevance of each indicator to the Cluster of Excellence. Cumulative entries of similar indicators are accepted if no further information on the individual recipients/items is provided (e.g. "3 ERC grants").

Renewal proposals only: These indicators do not have to be related to work carried out during the first funding period.

Estimation:

Strictly confidential
draft version

A.3 The 25 most important additional qualification indicators

Strictly confidential
draft version

Guidelines for A.4:

If the applicant university is proposing only one Cluster of Excellence, section 4.1 and section 4.2 can be combined.

Renewal proposals should include a description of the respective measures and expenditures of the first funding period in both subsections.

Guidelines for A.4.1:

If your university is proposing or jointly proposing more than one Cluster of Excellence with a university allowance, please indicate the other Clusters here and state the overall strategic aim of the proposals.

In no more than two pages, outline how the university intends to develop with the help of each university allowance and how governance at the university is to be strengthened. This description should be identical for all proposals submitted by a given university. In terms of content, the reasons given should also be compatible with any subsequent proposal for funding as a University of Excellence.

In the case of proposals submitted by university consortia, please include an explanation for each applicant university.

Guidelines for A.4.2:

In no more than four pages, please explain what strategic objectives are to be pursued at your university or jointly by the applicant universities with the aid of the university allowance if the proposed Cluster of Excellence is approved. What measures are envisaged by the applicant university/universities? A detailed breakdown of the planned usage of the university allowance must be submitted following approval.

Estimation:

A Appendix

A.4 Proposal for a university allowance

A.4.1 Overall concept of the applicant university/universities regarding strategic orientation and the university allowance

A.4.2 Envisaged use of the university allowance

Strictly confidential
draft version

Guidelines for A.5.1:

Please complete the following tables. Please do not provide any further information beyond the tables requested.

Guidelines for A.5.2:

In no more than a single page, please describe the effects of the coronavirus pandemic on the Cluster's work in the first funding period and, if applicable, any mitigating measures taken.

Estimation:

Strictly confidential
draft version

A.5 Data on the first funding period

A.5.1 Data on the first funding period

Table A.5.1: Total Expenditure by category

	2019	2020	2021	2022	2023
Totals per year in thousand euros					
Staff	3780	4480	5312	4906	5306
Professors	0	0	0	0	0
Junior research group leaders	0	0	0	0	0
Postdocs	308	636	608	393	586
Doctoral researchers	3111	3510	4134	4164	4314
Other research staff	361	334	570	349	406
Direct project costs (excl. research staff)	583	647	799	792	761
Instrumentation > €100,000					
Total expenditure					

Table A.5.2: Number of staff funded

	2019	2020	2021	2022	2023
Number of persons					
Professors					
Junior research group leaders					
Postdocs					
Doctoral researchers					
Other staff					

Table A.5.3: Expenditures for Structural Measures

Structural measures	Total* 2019-2023
Early-career researchers**	
Equity and diversity	
Research data and research software management; research infrastructures and instrumentation	
Management, governance, quality assurance	
Science communication, knowledge transfer and research-oriented teaching	
Collaboration with external partners	
Total	

* in thousand euros

**excluding salaries for doctoral researchers, Postdocs, Junior Research group leaders

Table A.5.4: Staff diversity – recruitment

	Number of persons recruited				total
	from applicant and/or participating institutions	from other German institutions	from institutions in Europe	from Non-European Institutions	
Professors					
Junior research group leaders					
Postdocs					
Doctoral researchers					

Table A.5.5: Staff diversity – gender

	Number of persons recruited			total
	female	male	diverse	
Professors				
Junior research group leaders				
Postdocs				
Doctoral researchers				

A.5.2 Effects of the Coronavirus Pandemic