The Integrated Fuel & Chemical Science Center

Adaptive Conversion Systems for Sustainable Energy Carriers & Chemicals

Renewal Proposal EXC2186

Contents

Nomenclature

Acronyms and abbreviations

5-HMF	5-hydroxymethylfurufural
AEM	anion exchange membrane
AESA	absolute environmental sustainability assessment
AI	artificial intelligence
AOR	ammonia oxidation reaction
AR	Associated Researcher
BCY	yttrium-doped barium cerate
BCZY	yttrium-doped barium zirconate-cerate
BECCU	bio-energy conversion with carbon capture and utilization
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
CEM	cation-exchange membrane
CEMC	cluster-expansion method calculations
CFO	Chief Financial Officer
CMP	Center for Mobile Propulsion
CNF	carbon nanofiber
CNT	carbon nanotubes
CO2RR	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
DAC	direct air capture
DAFC	direct ammonia fuel cell
DFG	Deutsche Forschungsgemeinschaft
DFT	density functional theory
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
EHL	elastohydrodynamic lubrication
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
fs-CARS	femtosecond Coherent Anti-Stokes Raman Spectroscopy
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
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
IR	infrared
ISPR	*in situ* product removal
ITMC	Institute of Technical and Macromolecular Chemistry
JARA	Jülich Aachen Research Alliance
KEAA	ketone-esters-alcohol-alkanes
LAS	laser absorption spectroscopy

LBV	laminar burning velocity
LCA	life-cycle assessment
LDM	low-degradation mode
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
OME	oxymethylene
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
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
TEM	transmission electron microscopy
TMFB	Tailor-Made Fuels from Biomass
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
The Integrated Fuel & Chemical Science Center
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 Con- version

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	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
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	Institute of Energy Technologies	

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(Continued)

No.	Principal Investigators	Location/ Institution	Field of Expertise	Position
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 Technical Chemistry	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. Mirijam Zobel*	Aachen, RWTH	Crystallography and X-Ray Spectroscopy	W3 permanent

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

* principal investigators who were 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)

Since the mid 20th century, crude oil has “fueled” the Anthropocene – literally through production of liquid energy carriers for mobility and transportation as well as by providing the crucial feedstock for the chemical value chain. The future will be renewable! Shaping a post-fossil era requires novel research concepts and breakthroughs in fundamental science to develop disruptive technologies as basis for a truly sustainable energy-chemistry interface within the planetary boundaries.

In this highly dynamic context, The Integrated Fuel & Chemical Science Center (FSC^2) 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. RWTH Aachen University and its strategic partners Forschungszentrum Jülich and Max Planck Institute for Chemical Energy Conversion integrate their competencies, methods, and infrastructures to understand, master, and design sustainable processes for harnessing renewable energy in molecular form for distribution, storage, and use on a global scale.

The interdisciplinary Competence Areas (CAs) spanning the molecular, device, and systems levels, successfully established with a focus on fuels and combustion systems for on-road mobility over the last five years in The Fuel Science Center (FSC), form the backbone of a unique research frame-work launching it to the next level as FSC^2. All research activities are allocated within five Strategic Research Areas (SRAs) stimulating disciplinary progress and fostering interdisciplinary integration. With the specific infrastructure of the partner institutions and the scientific profiles of the involved Principle Investigators, FSC^2 is ideally positioned to align groundbreaking science with focal technology options in light of systems analysis. Continuing efforts from the previous phase focus on fuel design for low-carbon and low-emission liquid energy carriers. Nitrogen-based substances such as Ammonia are included newly to asses critically their potential as molecular energy carrier and chemical building block. In addition to thermal energy conversion, electrochemical devices for recuperating chemically stored energy are studied and the applicability of molecular controlled combustion systems to existing vehicle is considered. The chemical value chain is explicitly addressed as a major area of application for novel synthetic pathways and catalytic processes. Analysis on a systems level is developed as integrative part to provide design criteria for sustainability and resilience within planetary boundaries.

2.2 German (max. 3000 characters incl. spaces)

Seit Mitte des 20. Jahrhunderts hat Erdöl das Anthropozän ”befeuer” – buchstäblich durch die Produktion flüssiger Energieträger für Mobilität und Transport sowie durch die Bereitstellung des entscheidenden Rohstoffs für die chemische Wertschöpfungskette. Die Zukunft wird erneuerbar sein! Die Gestaltung einer postfossilen Ära erfordert neue Forschungskonzepte und Durchbrüche in der Grundlagenforschung, um disruptive Technologien zu entwickeln, die als Basis für eine wirklich nachhaltige Energie-Chemie-Schnittstelle innerhalb der planetaren Grenzen dienen.

In diesem hochdynamischen Kontext generiert The Integrated Fuel & Chemical Science Center (FSC^2) grundlegendes Wissen und neue wissenschaftliche Methoden für die Entwicklung adaptiver technischer Lösungen zur Verwertung erneuerbarer Elektrizität und Rohstoffe in flüssige Energieträger und Chemikalien in einem systemischen Ansatz. Die RWTH Aachen University und ihre strategischen Partner, das Forschungszentrum Jülich und das Max-Planck-Institut für Chemische En- ergiekonversion, integrieren ihre Kompetenzen, Methoden und Infrastrukturen, um nachhaltige Prozesse zu verstehen, zu beherrschen und zu gestalten, die erneuerbare Energie in molekularer Form für die globale Verteilung, Speicherung und Nutzung nutzbar machen. Die interdisziplinären Competence Areas (CAs), die sich auf die molekularen, Geräte- und Systemebenen erstrecken und in den letzten fünf Jahren im The Fuel Science Center (FSC) mit Fokus auf Kraftstoffe und Verbrennungssysteme für den Straßenverkehr erfolgreich etabliert wurden, bilden das Rückgrat eines einzigartigen Forschungsrahmens, der als The Integrated Fuel & Chemical Science Center (FSC^2) auf die nächste Stufe gehoben wird. Alle Forschungsaktivitäten sind in fünf Strategic Research Areas (SRAs) eingebettet, die den disziplinären Fortschritt stimulieren und die interdisziplinäre Integration fördern. Mit der spezifischen Infrastruktur der Partnerinstitutionen und den wissenschaftlichen Profilen der beteiligten Hauptforscher ist FSC^2 ideal positioniert, bahnbrechende Wissenschaft mit fokussierten Technologieoptionen im Lichte der Systemanalyse in Einklang zu bringen. Die fortgesetzten Bemühungen aus der vorherigen Phase konzentrieren sich auf das Kraftstoffdesign für kohlenstoffarme und emissionsarme flüssige Energieträger. Neu hinzugekommen ist Ammoniak, um dessen Potenzial als molekularer Energieträger und chemischer Baustein kritisch zu bewerten. Neben der thermischen Energiewandlung werden elektrochemische Geräte zur Rückgewinnung chemisch gespeicherter Energie untersucht. Die chemische Wertschöpfungskette wird ausdrücklich als Hauptanwendungsbereich für neue synthetische Wege und katalytische Prozesse angesprochen. Die Analyse auf Systemebene wird als integraler Bestandteil entwickelt, um Gestaltungskriterien für Nachhaltigkeit und Resilienz innerhalb der planetaren Grenzen bereitzustellen.

3 Objectives of the Cluster of Excellence

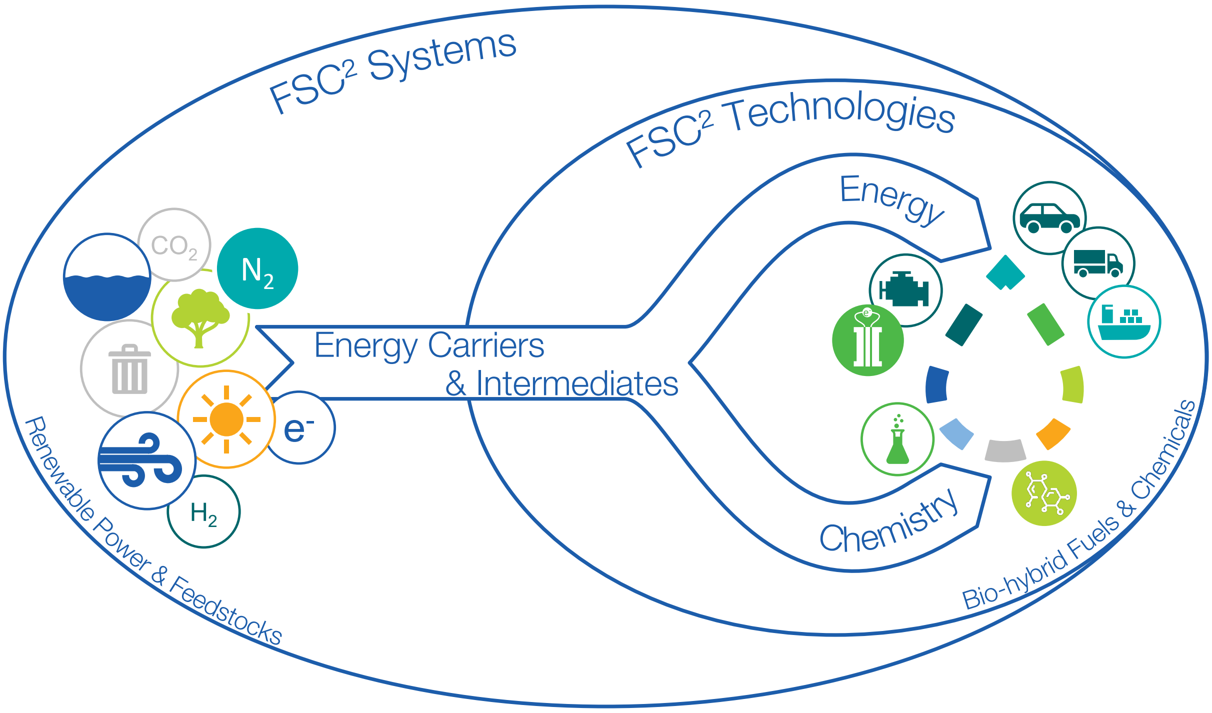
3.1 Background and Motivation

The urgently required reduction of greenhouse gas emissions, especially CO_2, 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 as cost-effective technologies for electricity generation(Lit). 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 (Lit). 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 (Lit).

Energy rich molecules – generated electrochemically or *via* green hydrogen - offer a key solution due to the high energy content of the chemical bond resulting in high volumetric and gravimetric energy density in liquid form. The integration of such energy carriers and 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 CO_2 emissions (Lit OPEC). Synthetic hydrocarbons, methanol, and ammonia are emerging as promising options and technologies for their generation from the abundant feedstocks water, nitrogen, CO_2 and biomass are demonstrated and deployed worldwide at rapidly increasing rate ([309]). 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 essential pillar for a closed anthropogenic carbon cycle. Innovative technological solutions and the assessment of their ecological, economic, and social consequences 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 (FSC^2) 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 chemical”.

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 (FSC^2)

Within The Integrated Fuel & Chemical Science Center (FSC^2), 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 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. FSC^2 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.

FSC^2 has its roots in the Cluster of Excellence (CoE) The Fuel Science Center (FSC). A unique interdisciplinary research culture was established overcoming disciplinary borders 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 structure

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 unchartered scientific territory. During this development, the synergistic potential of the studied production technologies for energy carries 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 FSC^2 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), FSC^2 is able to respond to the dynamic 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 fuel compatibility with existing vehicle fleets 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, FSC^2 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 both resilient to withstand and quickly recover from disruptions, and 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 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, CO_2-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 on 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 existing propulsion systems with the associated tight constraints regarding possible modifications. 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 N_2O.

3.3 Objectives

Based on the vision as well as resulting scientific challenges and key questions, FSC^2 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 & fuels via common intermediates to propulsion in existing & novel propulsion technologies; this is done by developing & combining cutting-edge methods from molecular design, propulsion equipment design, production process development, and machine learning.
Design of 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.
Concatenated bio-, chemo- and electrocatalytic transformations for bio-hybrid fuels and chemicals will be enabled 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-fuel based 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 enabled by fundamental understanding of the involved thermochemical and electrochemical processes.
Design of resilient and sustainable global conversion systems that integrate FSC^2 pathways, fuels, and chemicals with competing and synergistic pathways and products via systemic risks, stakeholder perspectives, policies, and sustainability criteria.
Structural Objectives
FSC^2 furnishes 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; it 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 renewal of FSC^2 through 9 reappointments of established lighthouse professorships, and 4 strategic new appointments as tenure track and lighthouse professorships in inter-faculty and inter-institutional frameworks 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 is accomplished through a comprehensive set of developmental measures and an individualized curriculum organized within FSC^2 Research School.
Fostering 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 (FSC^2) 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 of fuels and chemicals, and (iii) integrated design approach of conversion systems for sustainability and resilience on a global scale.
FSC^2 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 FSC^2 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 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.

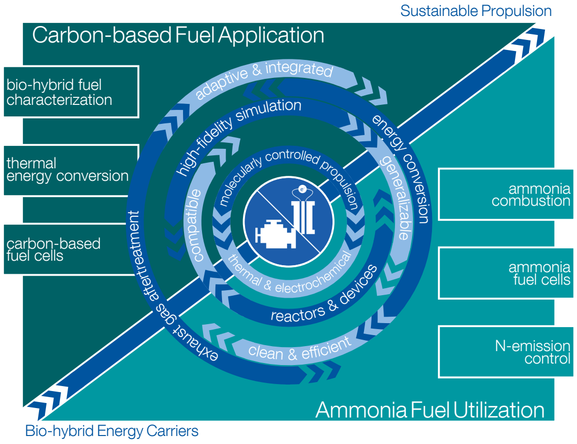


Figure 2: Joint methodologies and targets of SRA "Carbon-based Fuel Application" (SRA-CFA) and SRA "Ammonia Fuel Utilization" (SRA-AFU)

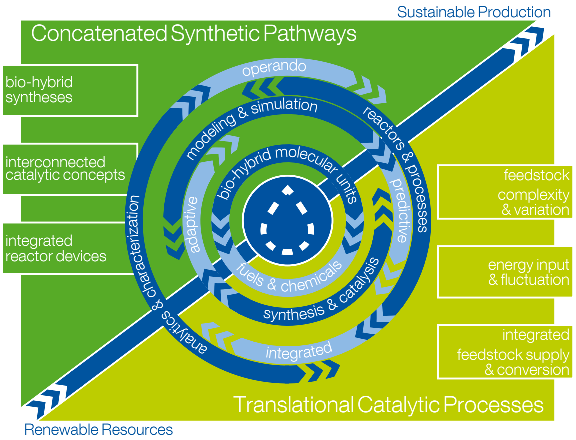


Figure 3: Joint methodologies and targets of SRA "Concatenated Synthetic Pathways" (SRA-CSP) and SRA "Translational Catalytic Processes" (SRA-TCP)

Two SRAs focus on production processes using non-fossil feedstocks and energy from renewable sources for the synthesis of biohybrid 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.

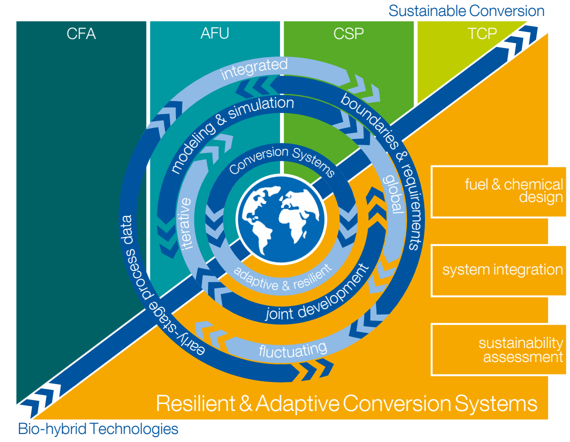


Figure 4: methodologies and targets of SRA "Resilient & Adaptive Conversion Systems" (SRA-RACS)

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, FSC^2 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 life-cycle assessment. The results of RACS are fed back to the other SRA consistently to enable an iterative research process within FSC^2 based on an ex-ante evaluation of developed process paths and fuels.

Working groups will be formed for common topics and techniques with the potential to crossfertilize 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 FSC^2 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 in the past. 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 then fundamental. In its new extension to chemicals, FSC^2 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 state.

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 CO_2-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 CO_2. Fostered by interdisciplinary collaboration from the molecular level through the modelling and demonstration of advanced devices to multifactorial systems analysis, adaptive production and propulsion technologies could be 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 FSC^2.
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 (REF, scientific objective 5). 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 CO_2 feedstocks. The integration of innovative bio-, chemo- and electrocatalytic methods for catalytic CO_2 conversion with biomass-derived building blocks opened unprecedented synthetic

routes to fuel targets beyond established products (scientific objective 1). 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 (scientific objective 4). Examples illustrating the interdisciplinary approach include the preparation of structurally versatile cyclic acetal bio-hybrid fuels by integrating biocatalytic alcohol formation and chemocatalytic CO_2 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 (REF). 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 50 % (REF). 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 (REF).

The detailed insights gained from such iterative studies were combined with advances in modelling and simulation as a basis for mathematical optimization methods across all levels (scientific objectives 2 and 6). This was successfully demonstrated for the holistic development of a bio-hybrid fuel blend made up of four different components. Using the process network flux analysis (PNFA) developed within the FSC, a blend with optimal CO_2 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 (scientific objective 3).

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 taken up and 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 (structural objective 3 and 4). The seamless integration of strategically planned appointments at various faculties and institutions demonstrates the pronounced structural effect of the cluster (structural objective 2). 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 (structural objective 1). The resulting tailor-made network was instrumental in establishing a number of important large-scale collaborative projects with strong translational components. (ReDiFuel, CatalAix, Helmholtz-Cluster Wasserstoff HCH2, Kopernikus Power-to-X, Carbon2Chem, NaMoSyn).

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 FSC^2.

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 FSC^2 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.

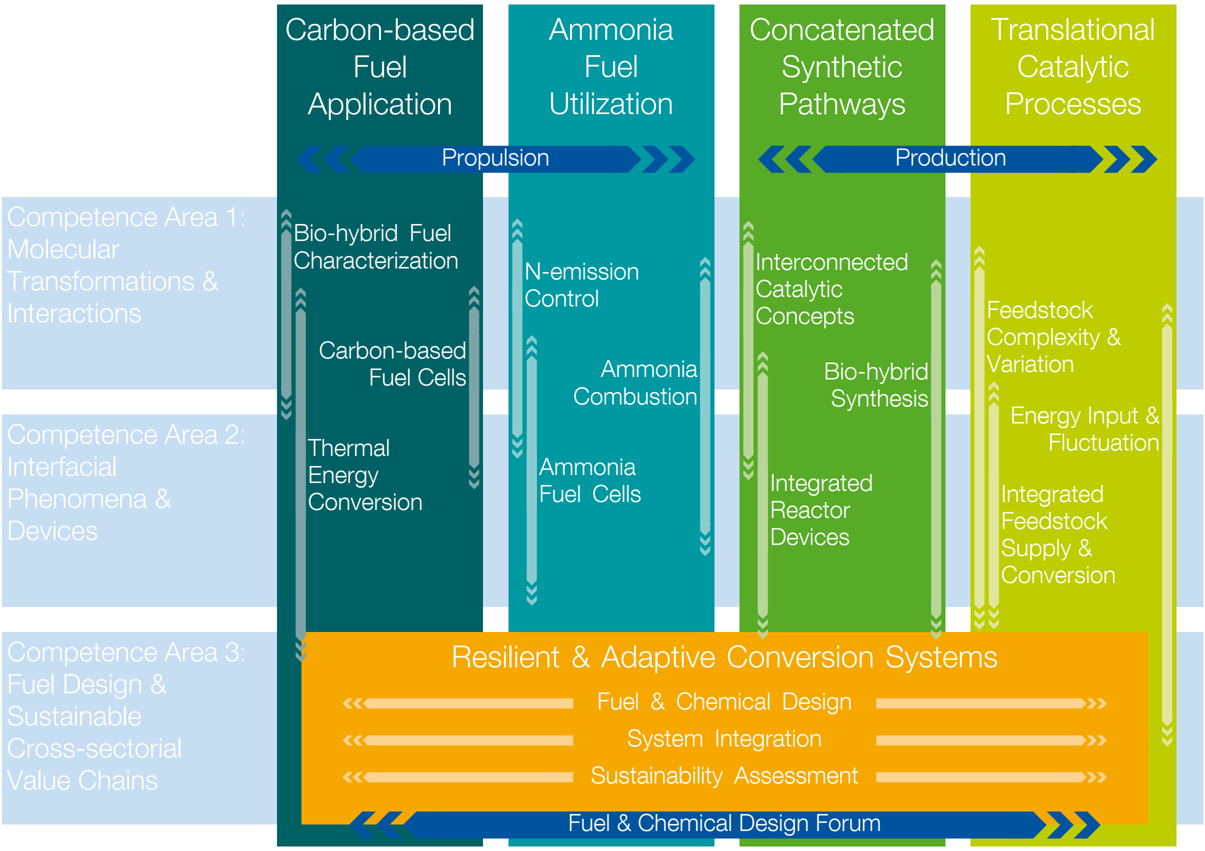


Figure 5: The integrated framework of the five Strategic Research Areas (SRAs) embedded within the Competence Areas (CAs).

Moving forward, all research activities and projects are allocated within thee 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 and Chemical Design Forum.

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.
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 FSC^2 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 Centur"-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 Section 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 FSC^2, 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 FSC^2 foresees the integration of further associated researchers de-

pending 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 FSC^2. 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 PI in the field of catalysis cover competences in heterogeneous catalysis (Palkovits), homogeneous catalysis (Bolm, Klankermayer, Leitner, Schoenebeck), and biocatalysis (Blank, Herres-Pawlis◊, 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 PI 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

Table 4.4.1: Cooperation matrix

■ main activity
□ supporting activity
◉ SRA coordination

		Carbon-based Fuel Application			Ammonia Fuel Utilization			Concatenated Synthetic Pathways			Translational Catalytic Processes			Resilient & Adaptive Conversion Systems		
Researcher's Institution & Main Competence	Strategic Research Area	Bio-hybrid Fuel Characterization	Thermal Energy Conversion	Carbon-based Fuel Cells	Ammonia Combustion	Ammonia Fuel Cells	N-Emission Control	Bio-hybrid Synthesis	Interconnected Catalytic Concepts	Integrated Reactor Devices	Feedstock Complexity & Variability	Energy Input & Fluctuation	Integrated Feedstock Supply & Conversion	Fuel & Chemical Design	System Integration	Life Cycle Assessment
Arning 💧 (RWTH)	Risk Perception & Communication		□	□			□				□			□	■	■
von der Aßen 💧 (RWTH)	Thermodynamic & Life Cycle Assessment	□	□	□				□	□		□		■	■	■	■
Backhaus 💧 (RWTH)	Environmental Impact	□	□		□		□			□	□			□	□	■
Blank (RWTH)	Metabolic Engineering of Microbes	□	□	□				■		□	■	■	■	□	□	□
Bolm (RWTH)	Catalysis for Organic Synthesis							■	■	□	□	□	□			
Boxx 💧 (RWTH)	Optical Diagnostics		■	■	■	■										
Eichel (FZJ & RWTH)	Electrocatalysis & HT Fuel Cells			■		■			□				□			
Greiff ◊ (RWTH)	Circular Economy & Sustainability										□			□	■	■
Herres-Pawlis ◊ (RWTH)	Bioinorganic Chemistry							■	□	■	■	□	■			
Heufer (RWTH)	High-pressure Ignition Kinetics	■	□		■		■									
Jupke (RWTH & FZJ)	Exp. Analysis & Model-based Reactor Design	□	□					■	■	■	■	■	■	□	□	□
Khetan 💧 (RWTH)	Multiscale Modelling of Heterogeneous Catalysis	□	■	■	□	■	■		□							□
Klankermayer (RWTH)	Translational Molecular Catalysis	□						■	■	□	■	□	■			
Kneer (RWTH)	Experimental Spray Characterization	□	■	□	■	□	■		■	■						
Lauterbach 💧 (RWTH)	Synthetic Microbiology			■				■	□	■	■	□	□			
Leicht-Scholten ◊ (RWTH)	Gender & Diversity in Engineering		□								□				■	■
Leitner (MPI CEC & RWTH)	Molecular Catalysis	□	□					■	■	□	■	◉	■	□		
Leonhard (RWTH)	Predictive Multi-scale Models	■	□	□	□	□	□	■								
Magnus 💧 (RWTH)	Biochemical Engineering	□	□					■	□	■	■	□	■	□		
Mayrhofer (FZJ)	Electrocatalysis			□		□		□	■	■	□	■	■			
Mechler 💧 (RWTH & FZJ)	Electrochemical Reaction Engineering	□		■		■		□	□	■	□	□	■	□		
Mitsos (RWTH & FZJ)	Process Design & Optimization	□	□	□				■		□	■	□	□	■	■	□
Palkovits (RWTH & FZJ)	Heterogeneous Catalysis, Nanostructured Materials	□	□				■	■	◉	■	■	■	■			
Pischinger (RWTH)	Combustion System Optimization	■	◉	■	■	■	■	□						□	□	□
Pitsch (RWTH)	Combustion, Multi-phase Flow	■	■	□	■	◉	■			■			■	□		□
Rother (FZJ & RWTH)	Chemo-enzymatic Syntheses	□	□					■	■	■	□	□	■	□		
Schmitz (RWTH)	High-pressure Fluid Analytics & Tribology	■	■	■	■	■	■			□	□			■		□
Schoenebeck (RWTH)	Catalysis at the Interface of Modeling & Exp.							■	■	□	■	■	□			
Schröder (RWTH)	Computational Fluid Dynamics	□	■	■	■	■	■									
Simon (RWTH)	Nanomaterials for Catalysis		□	□	□	□	■	□	■							
Venghaus 💧 (RWTH)	Decision Analysis & Socio-economic Assessment		□				□				□			□	■	■
Waldvogel ◊ (MPI CEC)	Electrosynthesis							■	■	□	■	■	□	□		
Walther (RWTH)	Planning of Sustainable Supply Chains		□					□			□	□	□	■	◉	■
Wessling (RWTH)	Electrocatalytic Membrane Reactors		□	■		■	□	■	■	■	□	□	■	□		
Wiegand 💧 (RWTH)	Magnetic Resonance of Catalysts							□	■	□	□	■	■	□		
Ziefle (RWTH)	Techn. Acceptance, Risk Communication	□	□				□				□			□	■	■
Zobel ◊ (RWTH)	Structure & Dynamics of Heterogeneous Catalyst							■	■	□	■	□				

in blue: associated PIs I ◊ new FSC member I 💧 strategic FSC appointment of systemic risk analysis (Arning💧, Ziefle), stakeholder incentives (Walther, Venghaus💧), and policy design (Venghaus💧, Walther). The results are combined with an environmental LCA (von der Aßen💧, Backhaus💧, Greiff◊, Leicht-Scholten◊) in an iterative design cycle to achieve resilient and adaptive fuel and chemical conversion systems that fulfill all aspects of sustainability. 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 FSC^2 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.

4.5 Detailed Description of the Research Program

4.5.1 Strategic Research Area: Carbon-based Fuel Application

PIs: Pischinger, Blank, Eichel, Heufer, Jupke, Klankermayer, Lauterbach, Leitner, Mechler, Mitsos, Palkovits, Pitsch ARs: Boxx, Kneer, Leonhard, Magnus, Schmitz, Schröder, Simon

The SRA "Carbon-based Fuel Application" (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 The Fuel Science Center (FSC) using novel bio-hybrid fuels and fundamentally new combustion systems like molecularly controlled combustion systems (MCCSs), which required dedicated engine designs. FSC-REF However, current propulsion systems will continue to have a significant share of the vehicle fleet in the decades to come. REF 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).
FSC^2 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

Heufer

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 life-cycle assessment (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 [1, 2, 3, 4, 5]. Such developments base on a detailed theoretical calculation of molecular dynamics (MD) [6, 7][246] with the highly recognized FSC-tool ChemTraYzer (CTY) (reviewed by [310, 311, 312]), on high-level quantum mechanics (QM) calculations of rate constants [8, 9], and thermodynamic data [10], as well as experimental results on laminar burning velocity (LBV) [11], ignition delay times (IDTs) [12], species measurements in flow reactors [13], and flame emissions [14, 15] 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 [16] and a comparative quantitative analysis of ammonia combustion models [17] demonstrated how knowledge of complex oxidation processes can be consolidated. Other popular approaches are automatic model generation [247][313] and parameter estimation [313].

Recent advances in data-driven ML, particularly in natural language processing (NLP) techniques [314, 315][18], 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 [316]. Owoyele and Pal [317] 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 [19] will be key to the further development of this method.

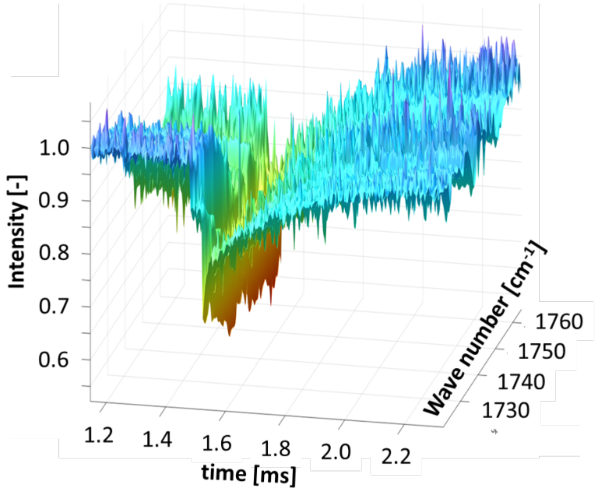


Figure 6: Measured time-resolved IR-absorption spectra during ethylformate pyrolysis

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 [5, 12, 3, 20, 21, 4]. For in-situ species measurements, a dual-comb infrared (IR) laser setup demonstrated its potential by scanning a wavenumber range 60 cm^{-1} with a time resolution of 4 μs [318][22]. 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

FSC^2 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, FSC^2 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 Tofhed 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. 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

Pischinger

The highly adaptive MCPSs are developed along a multi-stage, fleet compatible efficiency walk, which exploits the potentials of bio-hybrid fuels in terms of 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 fleet compatibility. For instance, increases of the CR cause increased surface-to-volume ratios, leading to increases of both the wall heat transfer and the emissions of unburned fuel. Hence, the near-wall effects will play a decisive role that forms a connection to the SRA “Ammonia Fuel Utilization” (SRA-AFU), in which the near-wall effects are also crucial due to the slow burning velocity of ammonia. Additional 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 already 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, in that 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. In this way, the combustion process was controlled by the reactivity share and the injection timings of the fuels. The continuous development of the MCCSs yielded an increasing η_i up to a maximum of $\eta_\mathrm{i} = 49.1\,\%$ by using CR = 19, see Figure 7a [23, 24, 25, 26, 27, 28, 29, 30]. For comparison, when using an active PC on an ICE with CR = 14, Peters et al. [319] achieved a maximum brake thermal efficiency of 42 % for a PC application, which is a proper value for current series ICEs. The engine-out emissions, especially in terms of the $\mathrm{NO_X}$-soot trade-off, were reduced when using the MCCS, representing near-to-zero pollutant emissions, see Figure 7b [29].

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 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. REF The charge motion and the mixture formation were investigated on an optically accessible ICE and

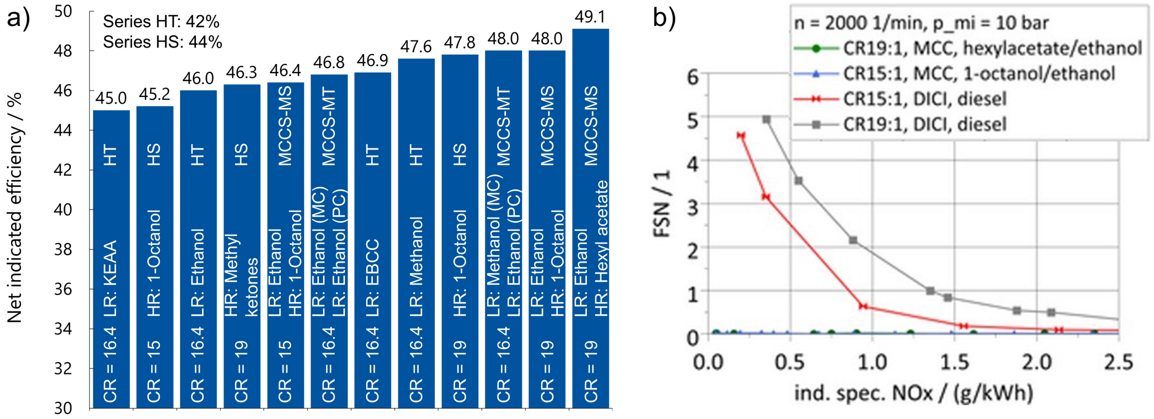


Figure 7: molecularly controlled combustion systems: a) efficiency walk; b) NO_X-soot trade-off.

in numerical simulations, which provided the basis for optimizing the injection timing for the MCCSs. REF For the MT, numerical simulations of the ICEs and optical investigations on an RCM revealed the timing of the PC jet ejection into the MC and the ignition of the MC charge by the jets, see Figure 8. REF For the flame quenching at the combustion chamber walls, a

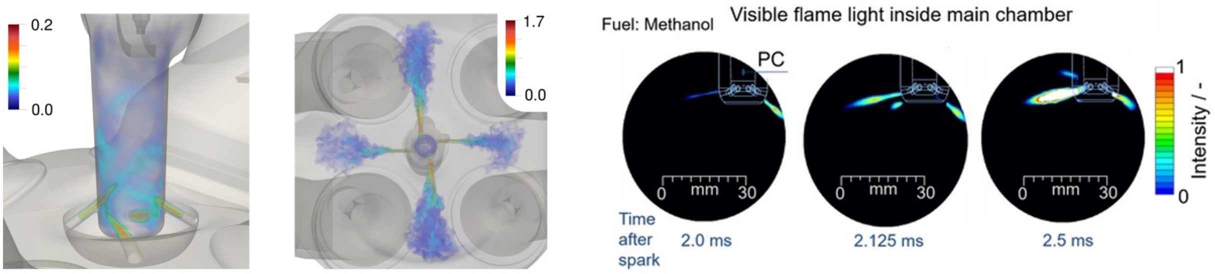


Figure 8: Numerical (left) and optical (right) investigation of pre-chamber jet ejection of the molecular torch.

methodology was developed to examine the resulting quench distance in optical investigations on an RCM using a dedicated quenching object, see Figure 9. When using coated quenching objects, the quench distance was reduced. In addition, investigations of coatings in a thermodynamic ICE revealed the reduction of both major HC species and CO [18]. 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 in inert atmosphere [31] (new paper 2024?).The MCCS-related investigations were not only performed for novel neat bio-hybrid fuels but also for fuel blends. The highly knock-resistant blend EBCC[1] slightly outperformed ethanol, whereas KEAA[2] achieved a similar η_i to 2-butanone, see Figure 7 [23, 27]. 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 [30]. In addition, the application of hydroformylated Fischer-Tropsch (HyFiT) fuels in a vehicle of the

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

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

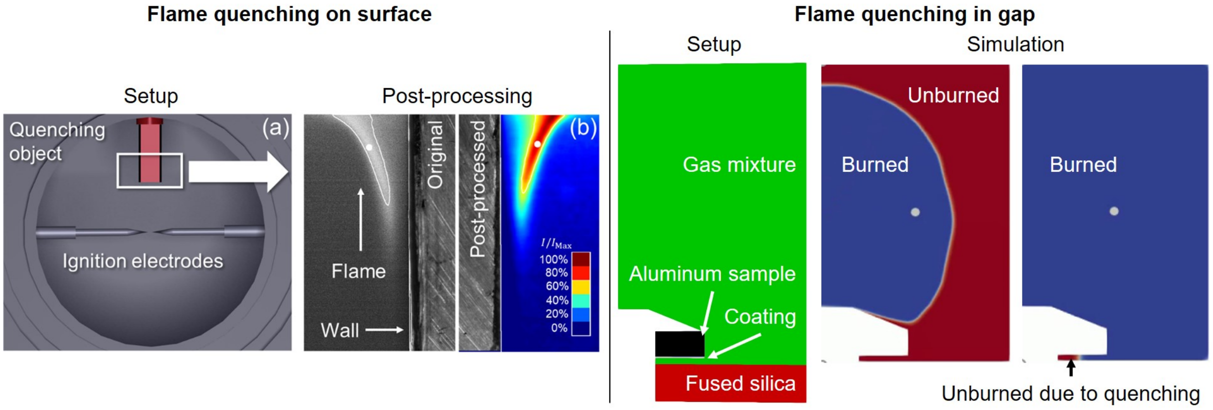

Figure 9: Left: flame quenching on (coated) quenching object in RCM [18]; right: simulation of flame quenching in (coated) gap.

current fleet reduced the engine-out particulate matter (PM) emissions by 55–70 % and the CO_2 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 %. REF 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 [32, 33, 30][Quelle: HyFiT] 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 [320].

Objectives

Based on the efficiency walk revealed in FSC, the SRA-CFA aims to develop a multi-stage efficiency walk in series applications 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 potential 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 still represent a retrofit solution that can be supplied to a wide range of the existing vehicle fleet. For this purpose, the SRA-CFA 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 (i) combustion concept, (ii) exhaust gas aftertreatment, and (iii) material & device compatibility.
By using the findings from the MCCS investigations in FSC, the combustion processes of the

MCPSs will be developed. Here, the challenge for a fleet-compatible engine design lies in the limited degrees of freedom, particularly with respect to the base engine (peak pressure limit), the crankshaft (stroke/bore ratio (s/D ratio)), and the cylinder head (gas exchange, charge motion, combustion chamber access). As possible degrees of freedom remain – with an increasing degree of effort – (i) the calibration and operating strategy, (ii) the ignition system, (iii) the injection system, and (iv) the piston.

Potential changes for the calibration settings of fleet vehicles are adjustments of the valve timing, the boost pressure, the injection strategy, and the EGR rate. The optimal calibration settings will be pre-evaluated using numerical simulations (Schröder). By carefully adjusting these parameters, the heat release in the engine shall be shaped depending on the applied fuel to increase the efficiency of the entire vehicle powertrain.

The MT will be applied to the fleet compatible MCPS as a retrofit ignition source (Pischinger). Hence, the MT 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. In particular, high lean operating limits in combination with high CRs shall be investigated to achieve maximum efficiencies.

For both the MT and the MS, injection systems featuring two separate injectors will be developed to enable the engine fueling with combinations of LR and HR fuels. Subsequently, the injection parameters will be optimized depending on the applied fuels to optimize the combustion process. In addition, the pistons will be replaced to enable an increase of the CR to increase the efficiency. However, this CR increase decreases the surface-to-volume ratio and causes crevices; thus, impacting the charge motion (Schröder) and potentially increasing the hydrocarbon (HC) emissions due to an increase of the quench distance. To reduce the HC emissions, combustion chamber coatings will be assessed fundamentally and in an engine (Pischinger, Heufer, Simon).

Associated with the retrofit fleet compatible solutions is the principal understanding of the relevant physical and chemical processes. Hence, experiments under well-defined engine-relevant conditions in CVCs and on an optically accessible single cylinder engine (SCE) will be performed (Boxx[3], Pischinger). These investigations aim to obtain accurate, high precision near-wall measurements of temperature and species concentrations under engine-relevant conditions with spatial resolution significantly smaller than that of the quench distance, using a 2D measurement system based on femtosecond Coherent Anti-Stokes Raman Spectroscopy (fs-CARS). This exciting new measurement capability, particularly in combination with well-developed techniques such as laser-induced fluorescence (LIF), Raman scattering spectroscopy, and chemiluminescence imaging will significantly enhance the understanding of piston-wall effects and flame-wall interactions with catalytic and thermal coatings under real engine conditions.

The remaining engine-out emissions of the MCPSs will be investigated using exhaust gas aftertreatment measures from FSC. To this end, the fundamental findings on MW-activated exhaust gas catalysis (Simon, [31] (new paper 2024?)) and 3D-printed catalyst carriers (Wessling,

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

Quelle linkhorst/CVT) will be combined into adaptive retrofit concepts and tested under realistic conditions on laboratory gas test benches (Pischinger). The experimental investigations will be accompanied by multi-scale simulations for a deep understanding of the underlying physico-chemical processes (Khetan[4]).

Prior to the experimental implementation, an initial assessment of the possible changes is carried out using the vehicle simulation tool chain established in FSC. With a virtual calibration, the vehicle including the hybrid powertrain operation and the exhaust gas aftertreatment will be optimized in terms of both the fuel consumption and the pollutant emissions (Pischinger), also enabling the integration of the vehicle into the LCA (see section 4.5.5.3) at an early development.

The integrated Fuel & Chemical Design Process (FCDP) is used as a starting point to identify fleet compatible bio-hybrid fuels and fuel blends (see chapter 4.5.5.1). Material and device compatibility of new fuel candidates will be investigated both numerically and experimentally (Schmitz). For the experimental investigation of the long-term compatibility of novel fuels without falsifying the significance of the results, new accelerated tests will be developed (Schmitz). To facilitate the process for the evaluation of the long-term behavior in terms of elastohydrodynamic lubrication (EHL), the comprehensive data base gained by accelerated testing will be utilized for a ML classification based on the molecular character of fuels and sealing materials. Since the simulation of long-term wear phenomena is related to high computational costs, fast-EHL approaches, which were developed in FSC, will be integrated.

Mechler

4.5.1.3 Carbon-based Fuel Cells

DLFCs show great potential as energy conversion systems with zero or near-to-zero environmental impact. Their advantage over hydrogen fuels cells is the use of liquid fuels, implying higher energy densities and a distribution within the existing fuel infrastructure. There is a large variety of possible fuels that can be converted for electricity generation. First reports even showed the use of different fuels in a single cell, allowing flexible fuel use for adaptive operation. For their further development, new catalysts and membranes are needed to reduce the noble-metal loading, lower cross-over, and reduce poisoning issues.

In FSC[2], 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.

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

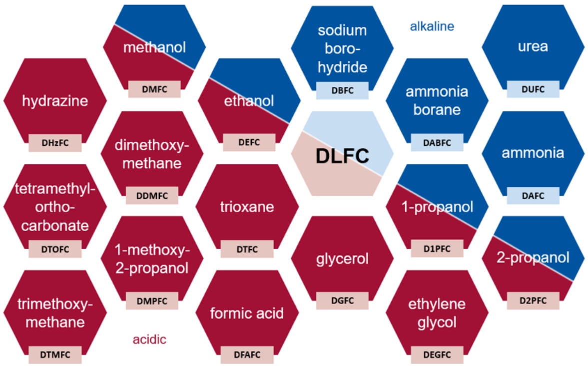

Figure 10: Illustration of most prominent DLFCs reported in literature

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 [321, 322]. In preliminary studies, we have identified candidates studied in the literature and characterized them regarding their thermodynamic as well as toxicological data (Figure DLFC_Overview, Mechler). 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 [322, 323]. Non-noble metal catalysts are more poison-resistant and furthermore significantly decrease the costs. For instance, carbon-based catalysts on the cathode and transition-metal based catalysts on the anode are promising alternatives [324, 325, 326].

The FSC^2 clusters vast experience in fuel cell catalyst development and characterization. For instance, we have studied non-noble metal and hybrid catalysts[248, 249, 250, 251, 252] (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 [253, 254, 255, 256] (Mechler, Mayrhofer) as well as magnetic resonance imaging (MRI) [257, 258], in-operando X-ray computed tomography (XCT) [259], and 3D transmission electron microscopy (TEM) [260, 261] (Eichel).

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 [327], and (ii) fuel blends can even have advantages over single fuel feeds in terms of performance and cross over [328].

For optimized catalyst-fuel interactions model-based optimization strategies are required. While various studies deal with the mechanistic investigation of specific fuel-catalyst pairs [REF], more generalized concepts that aim at tailoring the catalyst surface for a flexible fuel utilization are still missing. Here we can build on our capacities in the field of ab initio modelling of heterogeneous electrochemical reactions on oxides [262, 263], doped-graphene [264]as well as transition metal catalysts [265][...] (Khetan).

Furthermore, a tailored fuel design not only needs to investigate the reaction system, but also requires an understanding of the viability of the fuel production and utilization. Hence, a model-based screening of fuel candidates including the design and operation of the production and conversion processes is needed. Preliminary work covers the field of solvent [34] and process screening [35, 36], as well as integrated product and process design [37] (Mitsos). These approaches can be extended and applied to the application case of DLFCs. Moreover, we have experience in the modeling of electrochemical systems [38, 39] as well as in optimal design and operation [39], even applied to fuel cells [266]. For the supply of the required species property data for such methods, we can benefit from the prior work in the field of property prediction using ML [40].

Another significant challenge limiting the viability of DLFCs today is the high permeability of fuels through the membranes, which leads to reduced power output [329]. Surface and material modifications, and substitution of perfluorosulfonic acids (PFSAs) by hydrocarbon membranes, have shown to increase performance [329][267]. For anion exchange membranes (AEMs), the stability and conductivity still has to be improved for a successful implementation in real devices [268][330]. Additionally, the catalyst-membrane interface needs improvement in order to reduce overpotentials [331]. Alternatively, a bipolar membranes (BPMs) in forward bias can be used to operate anode and cathode in different environments [332, 333]. Within FSC^2 extensive background in membrane formation and characterization is available, including the modification of PFSAs-based cation-exchange membranes (CEMs) membranes to reduce methanol crossover [269, 270], hydrocarbon-based PFSAs substitutes [267], and micropatterning to increase the catalyst utilization at the catalyst-membrane interface [271]. Additionally, Wessling et al. have developed AEMs for direct methanol fuel cells [268, 272]. On a mission to increase the performance of reverse-bias BPMs numerous approaches were pursued in the past: the catalytic interface of the bipolar junction was engineered [273, 274], asymmetric BPMs were prepared for increased selectivity [275, 276] and modelled [277].

The application of reversible operation in reversible solid oxide cells (rSOCs) has demonstrated the potential to eliminate degradation [**?**]. This process involves alternating between fuel cell mode and electrolysis mode, which helps to prevent the formation of nano-cavities and other microstructural deteriorations [334]. Investigating regeneration strategies using short-term reverse operation will define optimized operation protocols that minimize degradation rates. Another key feature of rSOCs is their fuel flexibility, as highlighted by [335, **?**]., who demonstrated that rSOCs can operate with a variety of fuels, such as methane, diesel, and biofuels. However, studies also point out the associated challenges such as cooling due to endothermal reactions and carbon deposition [336]. System-level evaluation of rSOC systems is required to ensure that the benefits of fuel flexibility and reversible operation are realized in practical applications. A short-stack SOFC test conducted by FZJ demonstrated over 100,000 hours of continuous operation, showcasing the potential longevity of these systems. The challenges observed included chromium poisoning from cathodes, oxidation of metallic interconnectors, and non-linear degradation rates [**?**]. These factors complicate lifetime predictions and become increasingly complex when utilizing different fuels, underscoring the necessity for a holistic assessment of the underlying processes as well as robust operational strategies and modeling approaches. The TME institute has already investigated the add-mix of hydrogen to natural gas for a solid oxide fuel cell (SOFC) system, and a fuel-flexible single cell test bench is currently being commissioned. Initial results from the add-mixed operation have shown significant effects on the operating temperature of the fuel cell, necessitating the development of countermeasures through advanced and innovative control strategies.

For some applications microbial fuel cells (MBFCs) may 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. Also mechanisms observed in MBFCs can be utilized to optimize electrodes for DLFCs. Furthermore, a combination with heterogeneous cathodes in hybrid-fuel cells is possible for improved selectivity and performance. On the anode, lanthanide-containing methanol dehydrogenase (MDH) can be used, which can catalyze oxidation of alcohols towards the corresponding carboxylic acids in a four electron transfer step [337, 338]. However, 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 [278, 279](Lauterbach) and collaboration with cooperation partners for MDH-design [338], 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 FSC^2, 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 NH_3 are currently strongly discussed, there is a large variety of possible energy carrier molecules with differences in energy density, producability, storability, environmental impact, etc. Thus, the viability of these fuels will be accessed, not only considering their efficiency in the fuel conversion process, but also other aspects as the efficiency of their production process as well as their environmental impact (Mitsos, Leonhard). Therefore, the existing RNFA/PNFA framework will be extended to electrochemical systems, hence solving combined process design and operation optimization problems. ML will be used to cover a broad range of fuel candidates. This method can then be extended on tailored fuels, developed within the FCDF, with higher conversion rates, decreased poisoning and cross-over, or lower environmental impacts (cf. Chapter “Fuel Design”).

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). These calculations will be aimed at determining the potential-dependent free energies and reaction rates of reaction intermediates as well as contaminants in the presence of various co-adsorbates. 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 SRA “Concatenated Synthetic Pathways” (SRA-CSP) (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 (cf. state-of the art). This includes the consideration of material stability not only inside the fuel cell, but also in the whole fuel cell system. To ensure long-term operation of fuel cell systems without leakage, 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, AEMs as well as 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. To harness the potential of reversible operation in mitigating degradation in solid oxide cells, our research will build upon significant findings, as shown by Graves et al. [334], demonstrating how switching between fuel cell and electrolysis modes can prevent microstructural deterioration and extend cell lifespan. This mode switching eliminates reversible degradation and inhibits microstructural deterioration by maintaining a balanced distribution of oxygen vacancies and reducing particle migration, thereby mitigating the formation of nano-cavities, though the complete underlying physical processes are not yet fully understood. This strategy of operating cells in reversible mode not only prevents prolonged downtime but also establishes a low-degradation mode (LDM) that ensures sustained performance and reliability. Additionally, it facilitates the production of hydrogen, which seamlessly integrates into the assessment of different hydrogen add-mixes. To gain a fundamental understanding of these underlying processes, we will refine reversible cycling protocols through dedicated accelerated stress tests to establish optimal conditions that enhance performance while minimizing degradation, irrespective of the utilized fuel or fuel-hydrogen add-mix. The single cell test bench will be extended to operate in both fuel cell and electrolysis mode, thereby creating a test bench capable of being operated in both modes and a variety of carbon and non-carbon-based fuels. Advanced in-situ characterization techniques such as X-ray diffraction (XRD), TEM, and electrochemical impedance spectroscopy (EIS) will be employed to monitor changes in material structure and electrochemical behavior in real time. Computational modeling will support these efforts by simulating degradation pathways and enabling predictions that mitigate operational stresses on cell integrity. Understanding these processes, combined with the flexibility of reversible operation, will enhance the operational strategies of rSOCs systems. By switching between modes rather than shutting down the system, we can also avoid prolonged shutdown and start-up procedures while ensuring low lifetime degradation rates. These adaptive operating strategies, within the parameter space of fuel flexibility, emissions, efficiency, and low degradation, will enable the integration of rSOCs with diverse systems by fine-tuning operational temperature and pressure conditions to reduce thermal stress and overcome the challenges associated with cooling due to endothermic reactions without sacrificing efficiency. Continuous monitoring of voltage, current, power output, and degradation rates will provide critical data for real-time adjustment of operational parameters. Complementary gas composition analytics, including Fourier-transform infrared spectroscopy (FTIR) and non-dispersive infrared (NDIR), will also be employed. These techniques will further facilitate the development of tailored after-gas treatment strategies.. Minimizing polarization resistance through enhanced diagnostic tools will improve cell efficiency and operational life. Building on the findings by Forschungszentrum Jülich (FZJ), which demonstrated over 100,000 hours of continuous rSOCs operation, we will integrate these insights into our design and operation protocols. This long-term stability data will inform our development of new rSOC systems aimed at achieving similar or better longevity. We will hence investigate the fuel flexibility and reversible operation of state-of-the-art systems and their impact on efficiency, stability, and durability. Ensuring the practical applicability and scalability of rSOC technologies in real-world applications is crucial. We aim to integrate these advanced systems into existing energy infrastructures, including sectors such as heavy-duty transportation (trucks, aviation, maritime) and stationary energy systems (Pischinger).

For a full picture on available DLFC systems, also 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 [339]. 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.

4.5.1.4 Proposed Staff and Funding of SRA-CFA

Table 4.5.1.1: Proposed Staff in SRA-CFA[5]

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Staff category			**Number of persons**				
Professors	0	0	0	0	0	0	0
Independent junior research group leaders	0	0	0	0	0	0	0
Postdoctoral researchers	0	0	0	0	0	0	0
Doctoral researchers	11.5	11.5	11.5	11.5	11.5	11.5	11.5
Other staff	0	0	0	0	0	0	0

Table 4.5.1.2: Funding Request for SRA-CFA[6]

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Funding category		**Totals per year in thousand euros**					
Staff (Total for 4.5.1)	876	903	930	957	986	1016	1046
Direct project costs (excluding staff)	350	252	215	115	115	115	115

Continued on next page

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[5] Proposed staff funded by DFG solely comprises costs for scientific personnel for the planned research activities. Additional academic and other staff engaged in The Integrated Fuel & Chemical Science Center (FSC^2) but funded by institutional core support (Grundausstattung der beteiligten Partner) is listed in Table 6.2.1

(Continued)

	2026	2027	2028	2029	2030	2031	2032
Total instrumentation < €150,000	100	197	50	0	55	0	0
Total instrumentation > €150,000	156	150	0	0	0	0	0
Femtosecond Optical Parametric Amplifier	156						
Fuel Cell Test station for use with carbon-based fuels		150					

Instrumentation below 150 000 €

For the visualization of low-luminosity flames, such as very lean flames or hydrogen flames, in RCMs, a high-speed image intensifier is required (117 k€). 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€). In addition, by repeating experiments in RCMs and in STs for several times, the operating conditions cannot be maintained exactly. To investigate the combustion chemistry using multisampling of combustion gas, the procurement of a gas measurement system is required (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 fuels on newly developed ion exchange membranes for fuel cells, the experimental periphery for the measurements is required (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, high resolution laser-spectroscopic studies will be performed. Here, 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, the procurement of a femtosecond optical parametric amplifier (156 k€) is required. 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 (150k€).

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[6] For 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 Strategic Research Area: Ammonia Fuel Utilization

PIs: Pitsch, von der Aßen, Eichel, Mechler, Palkovits, Pischinger, Simon ARs: Boxx, Khetan, Kneer, Schmitz, Schröder

The SRA "Ammonia Fuel Utilization" (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 [340]. Also, its production is well understood and can be carbon neutral if based on renewable energy [341]. For utilization, NH_3 can be reformed to H_2 for use in internal combustion engines (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 [342] due to the higher overall efficiency potential [343]. 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 Strategic Research Area (SRA) is shown in Fig. 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 molecular torch (MT) concept in combination with reactivity tailoring by partial onboard or in-engine NH_3 reforming, and based on high compression ratio molecular spark (MS) engines with in-cylinder fuel staging. Novel injection methods for NH_3/H_2-blend injection will enable tailored mixing and staging

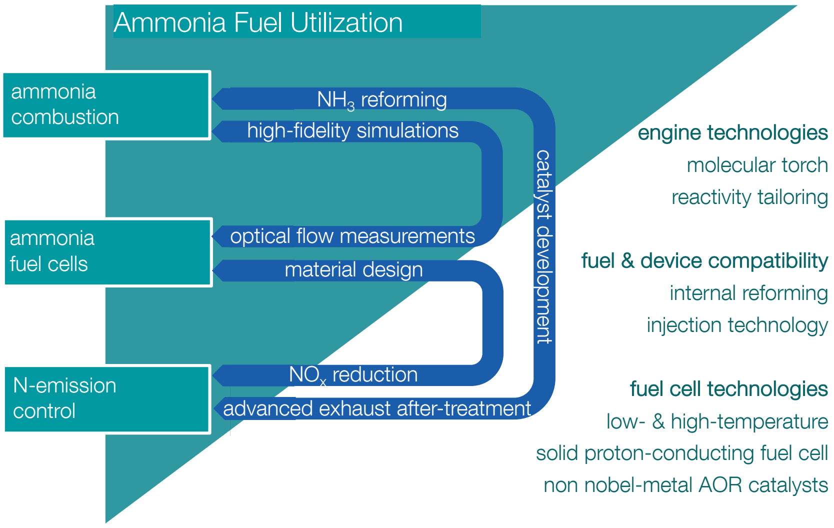

Figure 11: Structure of the SRA-AFU

strategies. The SRA-AFU will exploit all degrees of freedom to develop both retrofit and novel NH_3-engine concepts. 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 anion exchange membranes (AEMs). For direct NH_3 solid oxide fuel cell (SOFC), a challenge is the potential formation of nitrogen oxides. This can be mitigated 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 FSC^2. Strong 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

Pitsch

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 first project phase, 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.

Current State of Research and Previous work

Bio-hybrid fuels and their performance in ICEs have been systematically explored in the first project phase. 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 [344]. 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 [345, 346], cetane boosters [347], or H_2 [348, 349, 350]. 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 [351]. A 10% rate of NH_3 reforming, for instance, was found to enhance the engine's range of stable operating conditions significantly [352]. On the other hand, H_2-rich blends tend to increase NO_x and N_2O emissions [352]. 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][280], 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 [340]. 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 [348]. 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 $NH_3/H_2/N_2$-air flames poses significant challenges due to the unique intrinsic instability-induced highly nonlinear turbulence-flame interactions, as well as the complex flame-wall interactions and formation of nitrogen-containing pollutants [353, 354].

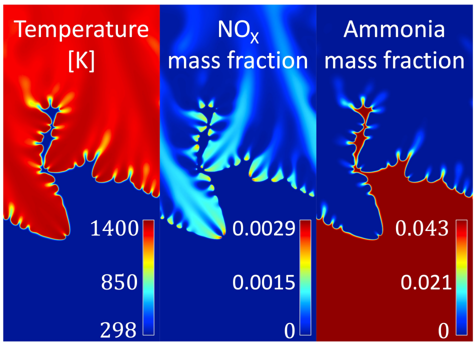

Figure 12: DNS of laminar NH_3/H_2/air flame with 40 mol-% H_2 showing intrinsic flame instabilities without which the flame would appear as a horizontal line.

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 [44, 17]. 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 Fig. 12. In addition, the research facilities already established in the first project phase provide a powerful toolset for investigating NH_3-based combustion. These include the thermodynamic and optical engines for performance, efficiency, and emission characteristics [24, 25, 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].

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 $NH_3/H_2/N_2$ 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 Fig. 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 machine learning (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.

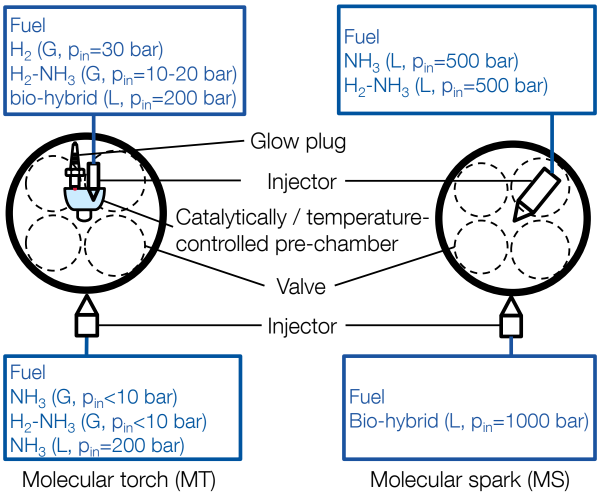

Figure 13: Ammonia engine concepts. 'L' stands for liquid, 'G' for gaseous, and 'p_{in}' for injection pressure.

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 MHBF 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 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.

Mechler/
Eichel

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

The Integrated Fuel & Chemical Science Center (FSC^2), we will investigate both low- and high-temperature fuel cells with highly active and selective catalysts that are resistant towards poisoning by 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.

Previous work

The concept of DAFCs has already been proposed about 50 years ago for both low-temperature [355] and high temperature applications [356]. Nowadays, the already utilized Ni-based electrodes show high NH_3 decomposition activity [**?**]. 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 [356]. 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 [357, 358, 359], this also causes new challenges, for instance, the need for improved catalyst activity [360, 361]. Typical materials for SPCFC electrolytes are yttrium-doped barium zirconate (BZY), yttrium-doped barium cerate (BCY) and yttrium-doped barium zirconate-cerate (BCZY) [357, 362]. Further doping with Yb further improves stability [358, 359, 363]. Within the cluster, we combine extensive experience in the field of material and cell development for SOFCs, both in fuel cell and electrolysis mode [281, 282, 283, 284, 285] (Eichel) with competences in the operation of fuel cell test benches [286] as well as fuel cell simulation addressing system performance, locally resolved electrochemical cell behavior, and mechanical stress distribution within the different cell materials [287, 288, 289] (Pischinger). First SPCFC separators have been developed with promising results at 600 °C [290] (Fig. 14), and under NH_3-operation [291].

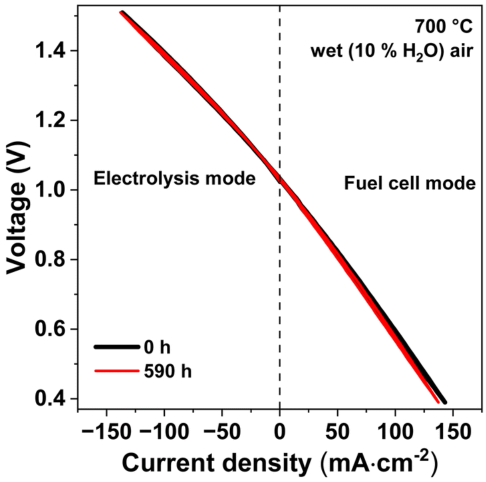

Figure 14: iV curves before and after 590 h in electrolysis operation of an electrolyte supported PNO/DNSYYb/Ni-BZY cell, showing the possibility of stable operation of SPCFCs.

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 [364, 365, 366, 367, 368]. 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 [369, 370, 371, 372, 373, 374, 375]. 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 [369, 375, 376]. 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 [250, 252, 251] (Mechler). 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 (Fig. 15).

Furthermore, the search for AEMs that are long-term stable in the NH_3 environment is still a challenge. Within FSC^2 we can built on long-term experience in membrane engineering of proton- as well as anion conducting ionomers, where a significant decrease of cross-over in direct liquid fuel cells (DLFCs) was proven [REFs to be added] (Wessling). 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, 52, 53, 54, 55] (Schröder).

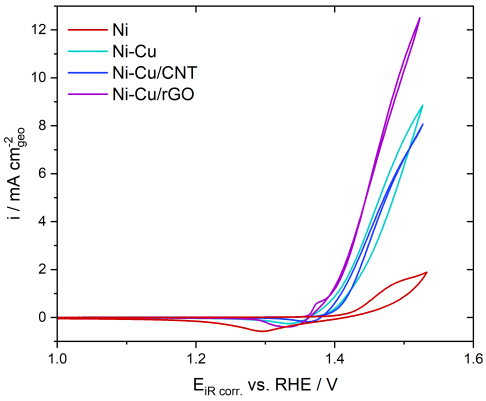

Figure 15: Rotating disc electrode measurements in 1 M KOH + 0.5 M NH_4OH for Ni- and Ni-Cu-hydroxides and the impact of supporting them on CNTs and rGO.

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. Fluroine-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 electrochemical impedance spectroscopy (EIS). Combined with advanced ex-situ and in-situ analysis (e.g., focused ion beam - scanning electron microscopy (FIB-SEM) tomography and high-temperature transmission electron microscopy (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 Fourier-transform infrared spectroscopy (FTIR) and non-dispersive infrared (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 fluorine-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. Further promising catalyst materials can be expected from insights developed in the SRA-CSP 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). These 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 such non-noble metal 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. Overall, 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 numerical 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.

Khetan

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 NO_x+N_2O removal at technologically relevant conditions. We will also explore unconventional methods like microwave (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

In the previous phase, The Fuel Science Center (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 [56, 57, 58, 47, 59]. 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 [59, 60, 61, 62][292]. 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 [60, 61, 62] [292]. However, these catalysts are mostly inactive for N_2O decomposition at such low temperatures. Our previous work [57, 58] and literature studies [377, 378] indicate 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 [379, 380, 381]. Thus, new low-temperature catalysts need to be developed with no or low precious metal content that allow for coupled DeNO$_x$-selective catalytic reduction (SCR) and N_2O decomposition under technologically relevant conditions [382, 383]. These conditions also include the inhibitory effects of O_2, NO_x, and H_2O, which are poorly understood [384, 385, 386]. 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 [349, 387, 388]. Conventionally, NH_3-slip catalysts utilized in automotive applications also form secondary NO and N_2O, thus posing further problems downstream. Therefore, either storing NH_3 or further reforming NH_3 into N_2 and H_2 with high selectivity are both sensible and necessary.

We have previously identified universal descriptors of catalytic activity [293] and rationalized the effect of strong metal/support interactions [294, 295] in doped oxides. Recently, we employed the ab initio energetic span model (ESM) to analyze N_2O decomposition activity on pure and hybrid catalysts [63]. 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 [31], as shown in Fig. 16. Using CO oxidation as a model reaction, this effort not 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.

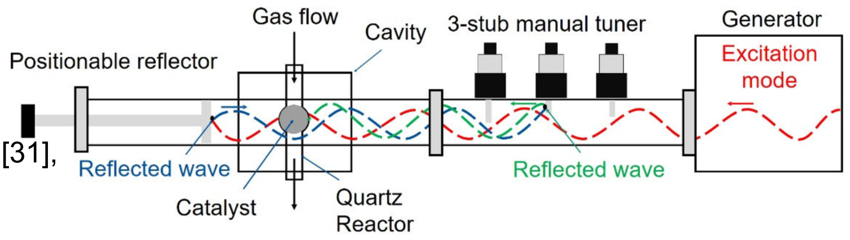

Figure 16: Schematic representation of the monomode MW-catalysis setup from our work [31] in which the MW-power directed towards the sample is maximized, while the power reflected back to the generator is minimized.

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 molecular dynamics (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 build upon our work [280] to identify and characterize promising catalysts for NH_3 reforming. Recent studies on bimetallic Fe/Ni- or Co/Ni-compounds have demonstrated comparable performance to Ru an Pd-based NH_3 reforming, and thus offer good starting points for developing a noble-metal-free system [389, 390, 391]. We will also explore the possibility of MW-driven NH_3 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 [392, 393] 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 [394] and Metal-Organic-Frameworks (MOF) [395] will be explored for their NH_3 storage capacity, including zeolites [296] [297] from our previous work. Going beyond thermally triggered release of stored NH_3, we will build upon our previous work [298] 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 ICCU, which is part of SRA-TCP.

For coupled DeNO$_x$-SCR and N_2O decomposition, we will develop transition metal-promoted zeolite catalysts, such as in our recent work on direct methane partial oxidation [64]. 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 [396, 397], 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 compressed sensing [398], 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 [399, 400] 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 [401, 402]. 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

	2026	2027	2028	2029	2030	2031	2032
Staff category	**Number of persons**						
Professors	0	0	0	0	0	0	0
Independent junior research group leaders	0	0	0	0	0	0	0
Postdoctoral researchers	1	1	1	1	1	1	1
Doctoral researchers	14	14	14	14	14	14	14
Other staff	0	0	0	0	0	0	0

Table 4.5.2.2: Funding Request for SRA-AFU

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff (Total for 4.5.2)	1067	1099	1132	1166	1201	1237	1274
Direct project costs (excluding staff)	305	250	150	150	150	150	150
Total instrumentation < €150,000	160	175	0	220	0	0	0
Total instrumentation > €150,000	156	415	150	0	0	0	0
Optical Parametric Amplifier	156						
Parallelized gas-phase reactor for Ammonia Decomposition		250					
Flex-fuel, reversible DL-SOFC single cell test bench		165					
Adaptation of HD cylinder head for thermodynamic investigations			150				

Instrumentation below 150 000 €

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 (60 000 €). 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 (100 000 €). For the optical investigation of the NH_3 combustion process, the optical single-cylinder engine from FSC has to be adapted (100 000 €). To investigate NH_3 DAFC applications, an NH_3 fuel cell test station has to be procured (120 000 €). 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 (100 000 €).

Instrumentation above 150 000 €

For the online analysis of the ammonia decomposition, a parallelized gas-phase reactor has to be procured (250 000 €). For the thermodynamic development of the NH_3 combustion process, a new cylinder head for the thermodynamic single-cylinder engine is required (150 000 €). 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 spectroscope (165 000 €).

4.5.3 Strategic Research Area: Concatenated Synthetic Pathways

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

Add short summary of SRA here

This Strategic Research Area (SRA) targets developing the catalytic toolbox necessary to generate a flexible bio-hybrid platform made of molecular building blocks that can be integrated into resilient material cycles [65]. On the molecular level, adapted catalytic systems should 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. Concatenated synthetic pathways take a system's approach instead. They target the integration of 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 over interconnected catalytic systems to integrated reactor concepts are in focus of this SRA.

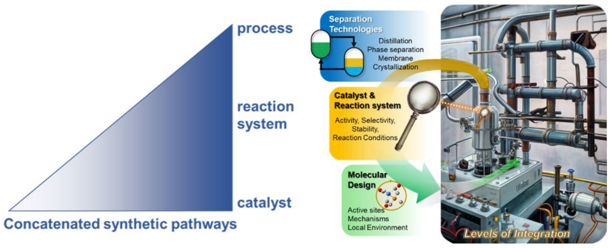

Figure 17: Holistic design of concatenated synthetic pathways considering the various options on the levels of catalyst, reaction system, and reactor and process design for an overall optimum.

Strategy and Structure of SRA

Concatenated synthetic pathways are considered on different length scales. At the molecular level, the focus is on catalytic transformations for bio-hybrid syntheses (Sub-Topic 1) that allow accessing the same products from different future carbon 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-Topic 2) enable at an optimum combination of catalytic transformations of various origin (bio-/chemo-

/electrocatalysts) and separations along a value path towards maximum resource efficiency at minimum energy needs and operational costs. Ultimately, several catalytic transformations together with the optimum separation technology are combined in integrated reactor systems (Sub-Topic 3) to provide the most desirable process concept.

Objectives for Main Part:
Concatenated synthetic pathways integrate both catalytic transformations as well as unit operations on the levels of catalyst, reactor and process enabling optimal resource and energy usage. Concatenated synthetic pathways provide the synthesis of bio-hybrid fuels and chemicals based on future carbon and nitrogen sources using renewable energies in a holistic approach.

4.5.3.1 Bio-hybrid Synthesis

Klankermayer

Add short summary here.
Detailed investigations of future scenarios indicate that only the integrated and flexible use of all available alternative future carbon sources and nitrogen will enable the chemical conversion of renewable energies on a scale relevant to the path to a resilient mobility and chemical sector [x]. The 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 a tailored access to the molecular motifs of the bio-hybrid platform based on the versatile raw materials. Catalyst development proceeds iteratively by combining forefront experimental and computations methodologies covering high-throughput synthesis and screening, operando analytics and data sciences.

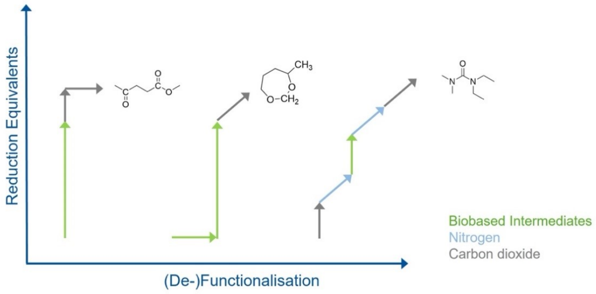

Figure 18: Access to the molecular motifs of the bio-hybrid platform based on the concatenation of catalytic pathways utilising different raw materials (biobased intermediates, nitrogen and carbon dioxide). The arrows indicate the tailored catalytic reduction and functionalization reactions or combinations thereof.

Previous work

Prior studies within the clusters of excellence Tailor-Made Fuels from Biomass (TMFB) and The Fuel Science Center (FSC) allowed establishing a broad toolbox of catalysts for the valorising biomass with focus on lignocellulose [REF] as well as CO_2 [66]. In these feedstocks, in contrast to fossil fuels, carbon is present in high oxidation state requiring selective defunctionalisation as well as selective reduction, for example through hydrogenation or direct electrocatalytic reduction. For the catalytic valorisation of CO_2, catalyst systems providing access to all almost all levels of carbon oxidation state could be developed by rational catalyst design [67, 68]. This includes new strategies for the reduction of CO_2 to formic acid as well as methanol with molecular [69] or solid catalysts [70, 71] providing flexibility with regard to operation in multiphase [72] reaction systems or even continuous fixed bed configurations. Major breakthroughs in the use of catalysts based on earth abundant 3d metals have been achieved. A nickel-based catalyst comprising the Triphos-ligand framework was shown to exhibit outstanding activity for formic acid formation [73]. The first catalytic system allowing direct hydrogenation of CO_2 to methanol based on manganese as active metal was designed based on a combination of experimental and computational methods [74, 75]. Utilising ligand structures as building blocks of materials, solid molecular catalysts composed of mono- and bidentate phosphines [76], pyridine, and triazine motifs [70] 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 H_2-D_2 exchange. By employing aberration-corrected scanning transmission electron microscopy, x-ray photoelectron spectroscopy and x-ray absorption spectroscopy, metal clusters, rather than single-atoms were confirmed as active species, providing new insights into the influence of gas atmosphere on metal speciation [77]. In contrast, for polyphosphines superior activity and selectivity of isolated metal species in CO_2 activation to formic acid was confirmed [78].

In contrast to formic acid and methanol as target products, the direct hydrogenation of CO_2 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 CO_2 hydrogenation on the formaldehyde level by in situ conversion into fuel and chemical targets. The concept was systematically established for the catalytic production of oxymethylene (OME) fuels [79] to the synthesis of for linear and cyclic acetates as bio-hybrid fuels by valorising various biogenic alcohols [80, 81, 82] or plastic waste [81]. The concatenation of bio- and chemo-catalytic steps was successfully demonstrated already for some selected cases by interdisciplinary collaboration of FSC teams. [83]. Though, many challenges remain open. Even with regard to the selective hydrogenation of CO and CO_2 to higher alcohols, methodologies to derive C_{2+} alcohols remain rare [84, 85]. In an innovative approach, Fischer-Tropsch synthesis to olefines was combined with reductive hydroformylation [86] A heterogeneous cobalt catalyst with high olefine selectivity could be integrated in tandem with thermostable cobalt reductive hydroformylation catalysts to produce a slurry-phase directly converting olefins to alcohols in a biphasic liquid/liquid system could be demonstrated. Immobilising the catalyst in a water phase for easy separation from the organic product phase enabled minimal Rh loss and continuous operation in a miniplant for more than 50 hours. [87]

Carboxylic acids beyond formic acid are highly interesting targets. Thus, a synthetic pathway to acetic acid via the formal isomerisation of methyl formate combining the two C1 products formic acid and methanol was established [88]. 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 [89]. Inserting CO_2 by carboxylation into nonactivated C-H bonds provides another attractive yet hitherto largely elusive catalytic transformation. Based on a computationally predicted Pd(II) complex, such a reaction could be realizes using simple and nonactivated arenes as starting materials. The potential of this catalytic reaction was demonstrated by the synthesis of veratric acid, an intermediate for pharmaceutical production, from CO_2 and veratrole [90].

Valorising bio-catalysis, microbial CO_2 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 to the industrial relevant platform chemical succinic acid were studied [91]. In another attempt, 72 different Ustilaginaceae strains from 36 species were investigated for their ability to (co-) consume the CO_2-derived substrates acetate and formate, contributing toward a carbon-neutral itaconate production. Ustilago maydis MB215 and Ustilago rabenhorstiana NBRC 8995 were identified as promising candidates for acetate metabolization whereas Ustilago cynodontis NBRC 7530 was identified as a potential production host using formate as a co-substrate enhancing the itaconate production. This proof-of-principle study clearly highlighted the potential of Ustilaginaceae biocatalyst candidates for carbon-neutral itaconate production. [92]

Electrocatalytic carbon dioxide reduction (CO2RR) [93] has also significantly evolved in recent years allowing access to e.g. CO, formic acid or ethylene [94]. For industrial relevant current densities at high selectivity an integrated catalyst and reactor design proved essential allowing to control local pH and ion strength. Despite the important role of the local environment at the electrodes, its assessment under true catalytic conditions, i.e. by in operando techniques, remains challenging. Multinuclear in operando NMR techniques were applied to CO2RR in aqueous $NaHCO_3$ or $KHCO_3$ over silver electrodes. 13C and 23Na NMR studies at different magnetic fields confirmed that the dynamic equilibrium of the electrolyte salt in solution, existing as ion pairs and free ions, decelerates with increasingly negative potential. This equilibrium affects the CO_2 resupply rate from the electrolyte. Substantiated by relaxation measurements, a mechanism was proposed where stable ion pairs in solution catalyse the bicarbonate dehydration reaction, which may provide a new pathway for improving educt resupply during CO_2 electrolysis [95]. Electrochemical real time mass spectrometry (EC-RTMS) presents another method providing real-time information to resolve transients occurring at dynamic interfaces. Applied to CO2RR during potential step or sweep experiments on pristine and in situ anodized copper, enhanced formation of several C_{2+} products over C1 products are tracked directly after copper anodization, with unprecedented temporal resolution. This creates exciting opportunities for resolving processes occurring at short timescales and even for enabling selective electrosynthesis under dynamic operation. [96, 95]

Regarding biomass, a broad set of chemo- and biocatalysts had already been developed within the cluster of excellence TMFB enabling the conversion of lignocellulosic biomass to a variety of intermediates or products [97, 98]. In FSC, the catalytic toolbox could be significantly broadened by utilising electrocatalytic biomass valorisation, e.g., for valorising 5-hydroxymethylfurfural [99]. Kolbe electrolysis was explored due to its potential to transform biogenic carboxylic acids to monomers and fuels [**?**], e.g., by electrochemical cross-coupling of biogenic di-acids allowing to flexibly tailor the fuel structures [100]. As overarching concept, anodic transformation at lower potentials compared to oxygen evolution reaction were explored potentially enabling electrocatalytic hydrogen formation at lower cell potentials companied by anodic formation of a valuable product [101]. An example comprehends glycerol electrooxidation, where the design of bimetallic PtCu electrocatalysts enabled superior selectivity to C_3 products which proved important for the economic potential of this technology [102]. Aiming for electrocatalyst prediction, comprehensive material characterisation highlighted covalency as electronic descriptor able to rationalize catalytic activity of transition metal perovskites in both oxygen evolution reaction (OER) as well as glycerol electro-oxidation but also in chemocatalytic NO reduction as well as N_2O decomposition [58, 103].

The Integrated Fuel & Chemical Science Center (FSC^2) Principal Investigators (PIs) also made first steps into integrating nitrogen functionalities in the valorisation of renewable feedstocks, e.g., via both chemo- and electrocatalytic amination and amidation of biogenic carboxylic acids. Comprehensive life-cycle assessment (LCA) and techno-economic analysis of the heterogeneously catalysed amidation of succinic acid to the monomer N-vinyl-2-pyrrolidone (NVP) was carried out. Indeed, LCA projected that bio-based NVP production reduces global warming impacts by 25–53% compared to compared to today's fossil alternative. [104]

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 [105, 106]. 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 strategy combining molecular and nanoparticle sites on a single support opens the way to the development of multifunctional catalytic systems capable of performing complex reaction sequences in one pot. [107]

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 19). 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 modelling 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 (see Figure X). Building upon the previously demonstrated access to compounds in the formal formaldehyde oxidation state, direct catalytic transformations e.g. by CO_2 reduction to formaldehyde and derivates will be in the focus. Research objectives comprehend methodologies to provide free formaldehyde utilising chemo- as well as bio- [108] and electrocatalysis (Klankermayer, Leitner, Mechler, Wessling). Formaldehyde corresponds to the same formal reduction level as carbohydrates and hence can be envisaged as attractive target as C-source for microbial transformations (Blank). Inspired by the cluster's previous success regarding in situ chemical transformation to formaldehyde derivates, the synthesis of linear and cyclic acetals will be extended and further developed providing input for activities 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 [109, 110, 111], the platform will serve as a starting point for new catalytic approaches towards C-C bond formation (N.N.).

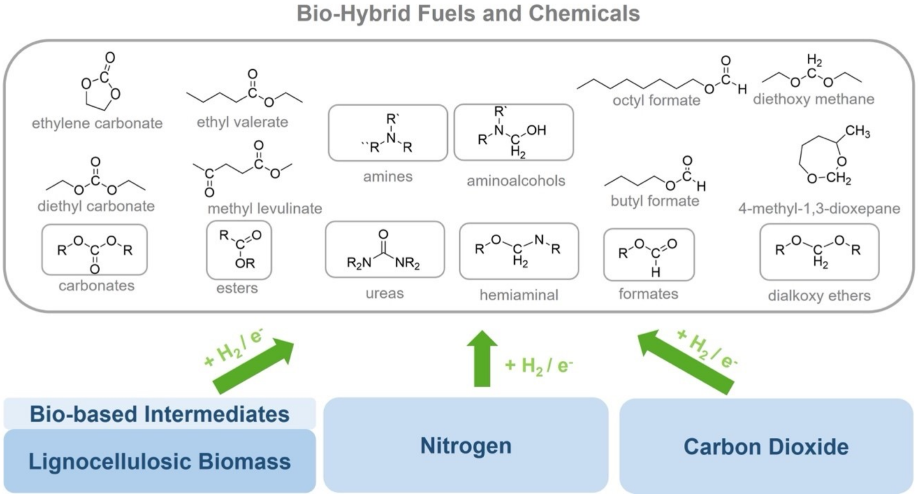

Figure 19: Catalytic toolbox for flexible access to bio-hybrid fuels and chemicals enabled by the sustainable formation of C–C, C–H, C–O, and C–N bonds.

Tailored catalytic transformations using the formaldehyde platform towards the synthesis of nitrogen containing compounds will be in focus also. This includes selective synthesis of aminals in analogy to the acetals. Novel N-methylation reactions (catalytic Eschweiler-Clarke methylation) based on CO_2 instead of formaldehyde can also be envisaged. A flexible catalyst platform

was demonstrated recently in FSC 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 functionalized copper NHC complexes for the A3 coupling and ruthenium nanoparticles for selective hydrogenation [REF].
Beyond formaldehyde, further approaches of C-C and C-N bond formation present major focus points of FSC^2 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 CO_2 valorisation. 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 to fuels, blends and valuable chemicals.
Building upon a mechanochemical activation of Mg and subsequent reaction of the in-situ generated organometallic reagent with CO_2 [Int1], N_2 activation by Ti in presence of reductants such as Mg will be studied. Ultimately, novel approaches to N_2 fixation as well as a direct activation of both N_2 and CO_2 will be explored in FSC^2 (Bolm, Wiegand, Zobel).

To achieve the indispensable advance in catalyst development, tools of automated catalyst synthesis, high-throughput screening, operando analytics and artificial intelligence (AI)-added data evaluation are valorised targeting accelerated development and ultimately catalyst prediction. For catalyst prediction, Schoenebeck group showcased how machine learning methods can be used to accelerate identifying catalyst design of previously unknown dinuclear Pd catalysts v [112, 113, 114, 115, 116, 117]. In FSC^2, 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 couples with automized catalyst synthesis platforms as key step for fully integrated workflows [118, 119, 120].
Accordingly, methodologies for parallelized and high-throughput testing together with the necessary data management and evaluation as already developed e.g. in electrocatalysis [121, 122, 123], will be extended to the other catalysis disciplines. Operando-analytics present a crucial element of knowledge-based accelerated catalyst design. Recent work on metal nuclearity under reaction conditions emphasise the highly dynamic nature of active sites under relevant reaction conditions [77]. Supervised learning (Examples)
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, modelling, 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. On the other hand, a new professorship will be established at the interface of chemistry, mechanical engineering and computer science (W3 Lab Automation and Chemical Robotics),

to enable developments in this fast-growing area of cutting-edge research that shape the international state of research.

Rother

4.5.3.2 Interconnected Catalytic Concepts

Add short summary here.

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, novel catalysts with several functions shall allow 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. These advantages include not only effective synthesis to high product concentrations with high purity and high step- as well as atom economy, but also the lowest possible energy input and therewith increased (eco-)efficiency. Accompanied by an integrated holistic design of energy- and resource-efficient separation technologies, a global 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 (fed-)batch and continuous reactor designs (see X.Y) are available for modular, flexible combinations. The outstanding element of this FSC^2 approach is the techno-economic overall balancing of the process including the catalytic reaction sequence as well as separation.

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. In general, bio-catalysis works best under aqueous reaction conditions and moderate temperature, while chemo-catalysis often operates in organic solvents at elevated temperature and pressure. Electro-catalysis allows direct use of renewable energy and can operate both in aqueous and organic media, but requires suitable electrolytes for sufficient charge transfer. To valorise 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 [73]. 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 makes this approach unfavourable [124]. 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 [125, 126]. In an alternative approach to overcome the separation challenge, whole-cell and enzyme catalysis were combined. A yeast-based acetaldehyde production with in situ gas stripping and capture was used [127]. Due to the high vapor pressure of acetaldehyde, this compound 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 [128]. Subsequently combined with chemocatalytic carbon dioxide incorporation in the formaldehyde oxidation state, cyclic and linear acetals become accessible broadening the available bio-hybrid chemical platform [25]. This concatenated synthetic pathway clearly exemplifies the potential of the integrated development concept of alternative production routes to minimize downstream costs and make sustainable production paths more competitive.

Recent advances for chemocatalysis in biological media [129] and biocatalysis in unconventional media [130] show 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 g L^{-1} h^{-1}, efficient with > 90 % theoretical yield, and the product can accumulate up to 150 g L^{-1} [131]. Still, starting from glucose even at 100 % theoretical yield, every third carbon atom is lost as CO_2 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 [132, 133]. To increase the atom economy – in this case for valuable carbon – of bioethanol fermentations, CO_2 might be directly uptaken. Within the FSC, Guntermann and Mengers et al. explored this by converting the microbial-produced waste-CO_2 in a 1-step, 1-pot approach [134]. Molecular ruthenium complexes are known to catalyze H_2-driven CO_2 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 [135]. After conflating the reaction conditions, the bioethanol fermentation was carried out in a high-pressure reactor under 120 bar of H_2 pressure simultaneously coupled with a Ru-catalyst residing in a tetradecane phase converting CO_2 and H_2 to formate. Ultimately, over 26 % of the nascent greenhouse gas 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 CO_2 output of 50 Mt a^{-1}, although minuscule compared to 31,900 Mt a^{-1} from fossil fuels [136], could mean a CO_2-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 [137].

Objectives

The objectives comprehend (i) directly integrating downstream processing into the design of concatenated transformations to achieve pathways with lowest possible energy demands and environmental footprint, (ii) combining catalysts of all types for conversion of future substrates into most economic and ecologic efficient processes. For this purpose, compatible reaction systems are designed. (iii) For optimal step and atom efficiency, multi-functional catalysts with several activities are designed; (iv) techno-economic overall balancing of the process including optimal reaction parameter prediction and verification are included.

Work Program

An important aim are integrated processes combining challenges in catalysis and downstream processing. Conventionally, sequential conversion and separation along a reaction sequence involves incorporating separation technology after each reaction step to purify the intermediate to the required purity of the following stem. While providing flexible process operation, this approach often results in costly separation tasks. To address this, energy efficient separation techniques for polar compounds from polar solvents will be explored including membranes, reactive extraction, or adsorption. To this end, experimental investigation as well as modelling of binding and reaction mechanisms in novel reactive separation systems consisting of tailored solvents (e.g. terpenoids) and adsorbents (e.g. functionalized boronic acid derivates) will be performed (Jupke, Palkovits) as well as characterization of novel membranes (Wessling). Specific examples comprehend reactive extraction e.g. for separating carboxylic acids from fermentation broths or amines from reaction mixtures. In addition, adsorptive techniques will be developed to separate valuable e.g. diols from aqueous solutions. In the next step, integrating transformation and separation is targeted. To effectively evaluate separation strategies, early-stage overall process design and optimization are applied. A major challenge is that at an early stage of development, there is only limited experimental data available as basis for analysis. FSC^2 overcomes 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. By identifying key factors and bottlenecks in an early stage of development, the full potential of interconnected catalytic system can be valorised (Jupke, Mitsos).

On the reaction level, traditionally, individual transformations and their respective reaction conditions (solvent, temp. pressure, etc.) are optimized individually hampering an integration along the reaction cascade. In compatible reaction systems, reaction sequences involving different catalytic transformations are enabled within a tailored reaction system enabling close integration. FSC^2 therefore focusses on smart solvent choices for multiple consecutive conversion steps without solvent change facilitating an efficient sequence. This holds true for the combination of each reaction step, but also for the combination of reaction and product separation (see below). Challenges comprehend identifying compatible solvents including model-based methodologies [REF] and optimizing the trade-off between the reaction steps, especially when the catalysts are of different origin (bio-, chemo-, or electrocatalysts) and evolved or optimised in their defined environment.

Examples on solvent selection (Andreas/Dörte Dioxolane)

To design truly novel, efficient processes from substrates of the future with minimal footprint, FSC^2 will now extent 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 ecologic 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 synthesised based on microbially produced butanol and aromatic compounds (from second generation feedstocks) ligated with formaldehyde from CO_2 fixation. From these intermediates, a set whole of products like diols, dioxolanes and amino alcohols will be accessible by further diversification with enzymes and chemocatalysts. In sum, 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 optimisation of the overall synthesis pathway, including downstream processing. (Klankermayer, Leitner, Palkovits, Herres-Pawlis, Rother, Blank, Lauterbach, Magnus, Jupke, Walther, Heufer); In a second example

Beispiel Regina zu Bio-/Elektrokatalyse! (z.B. Aminierungen von Aldehyden/Ketone)

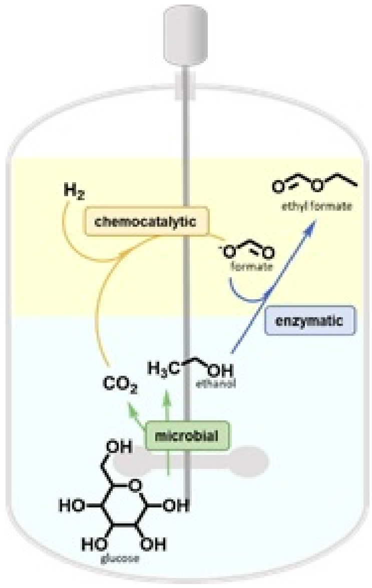

Figure 20: Combination of microbial, chemocatalytic, and enzymatic catalysts for the integrated synthesis of ethyl formate from biomass and CO_2 in a one-pot, two liquid-phase reactor.

4.5.3.3 Integrated Reactor Devices

Jupke

Add short summary here.

Reactor design plays a pivotal role in the conversion of sustainable hydrogen, carbon, and nitrogen sources for the formation of C–C, C–H, C–O, and C–N bonds of functional molecules. Leveraging a toolbox of chemo-, bio-, and electrocatalytic conversion steps, these concatenated catalytic pathways incorporate multi-phase reactors. To achieve high yields, novel intensified reactor devices are utilized, enhancing the efficiency and effectiveness of the conversion process. Thus, adaptive, flexible, autonomous, and self-optimizing innovative conversion apparatuses are needed.

Tailored approaches are required to understand and optimise the multi-phase flow dynamics within each reactor type, reflecting the complex interplay between design, operation and the specific characteristics of the chemical processes involved. To advance the envisaged modular units, we will break them down into smaller repeating sub-units, such as tubular or 3D printed entities, designed for conversion and separation processes through molecular functionalisation. At the smallest scale, fundamental molecular phenomena will be studied and control mechanisms developed. This hierarchical approach will integrate knowledge for the design of adaptive devices using multi-scale fabrication methods. Such integration across length scales and disciplines requires collaborative efforts leading to effective optimisation cycles.

Previous work

In FSC, (electro-)chemical reactors were designed to consider three essential elements (i) sequentiality and parallelization of modular functional units, (ii) control of modular multi-phase flow and (iii) integration of multiple functions such as controlled creation of reactive interfaces and product removal.

In biochemical synthesis, *in situ* product removal (ISPR) plays a crucial role to overcome product inhibition. An example for biochemical conversion with in situ product removal in an innovative reactor concept is the production of methyl ketone in a multi-phase loop reactor [138]. This reactor as a one-pot reactor combines biochemical conversion with a corresponding separation sequence without simultaneous loss of yield [139]. Further, ISPR concepts can work the other way around where the biotransformation acts as the product sink for a chemical reaction system. To this end, we implemented a chemical and biochemical puzzle, combining homogeneous chemical and biochemical reaction. The aim was to investigate the chemical conversion of H_2 and CO_2 into formic acid and subsequent extraction into an aqueous phase, enabled its biotransformation into itaconic acid [92, 140]. With the proposed integrated ISPR concept, the carbon dioxide emission of the microbes can be used again as educt for the chemical conversion [134].

Pure liquid phase chemical reactions can also benefit from applying ISPR and merging reaction as well as separation steps in an integrated reactor concept. This involves introducing a second liquid phase into the chemical system, creating a multiphase system consisting of two liquid phases. If one of the reactants is gaseous, mass transfer from the gaseous to the liquid phase must also be considered, resulting in a complex three-phase vapor-liquid-liquid system. By using ISPR in various adaptive design frameworks, side reactions can be reduced and the equilibrium limitation in the reaction can be overcome as far as possible to achieve higher yields and selectivities. Within the previous FSC cluster, an integrated reactor network consisting of a biphasic homogeneously catalysed hydrogenation of carbon dioxide to formic acid was enhanced by ISPR [141, 72]. The chemical conversion of diols to 1,3-dioxolanes was also investigated. To address the complex reaction system characterised by equilibrium constraints and CO_2 conversion, process intensification involves *in situ* extraction, incorporating a non-polar phase to create a complex vapor-liquid-liquid integrated reaction and separation process.

A biomass-based process from fructose via 5-hydroxymethylfurufural (5-HMF) to furandicarboxylic acid (FDCA) was significantly enhanced by process intensification and integration [142, 143]. The design and operation of a continuous multiphase 5-HMF reactor, where in-situ extraction reduces by product formation and product degradation, was assessed by a simulation model to gain fundamental knowledge on the process and enable adjustment of operating conditions [34, 144]. The process was further intensified by a consecutive electrochemical conversion of 5-HMF to FDCA. By directly feeding the diluted organic 5-HMF stream from chemical conversion to a biphasic electrochemical reactor, the integrated process eliminates the need for an intermediate purification step, as depicted in Figure 21 [145]. The efficiency of electrochemical reactors can be increased by the so-called paired synthesis of two value-added products at both, anode and cathode. In a recent work we have demonstrated how to systematically design such a paired electrolysis of HMF oxidation and acetoin reduction to obtain high conversions and stable process conditions. We demonstrated that an additional process intensification by direct electrochemical conversion of acetoin-rich fermentation supernatant is feasible [145], but trace metal impurities decrease the selectivity. These can be overcome by a resting cell approach in the fermentation step [146].

Another way to improve electrochemical reactors is by using the dynamic extension of electrochemically active surface area by flow electrodes or slurry electrodes [147, 148].

Tubular electrodes promise modular reactor concepts with high surface to volume ratio. 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 [149] enables, in combination with steering the process conditions, a high degree in control over the reactor's selectivity. [149] In a next step, several tubular electrodes were integrated into one re-

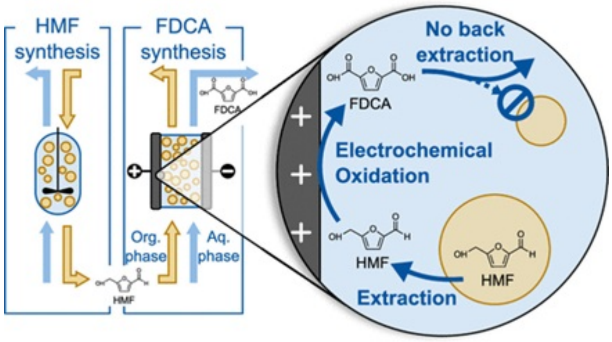

Figure 21: Integrated conversion of fructose to FDCA in a biphasic systems comprising chemical and electrochemical conversion.

actor, which enable swift scale-up via numbering-up (Figure 22) [150, 151]. We also exploited the high degree of freedom in design by 3D printing triply periodic minimal surfaces (TPMS) entities, and to integrate two functions into the electrode domain: high active surface area and enhanced mass transfer [152, 147, 153, 148].

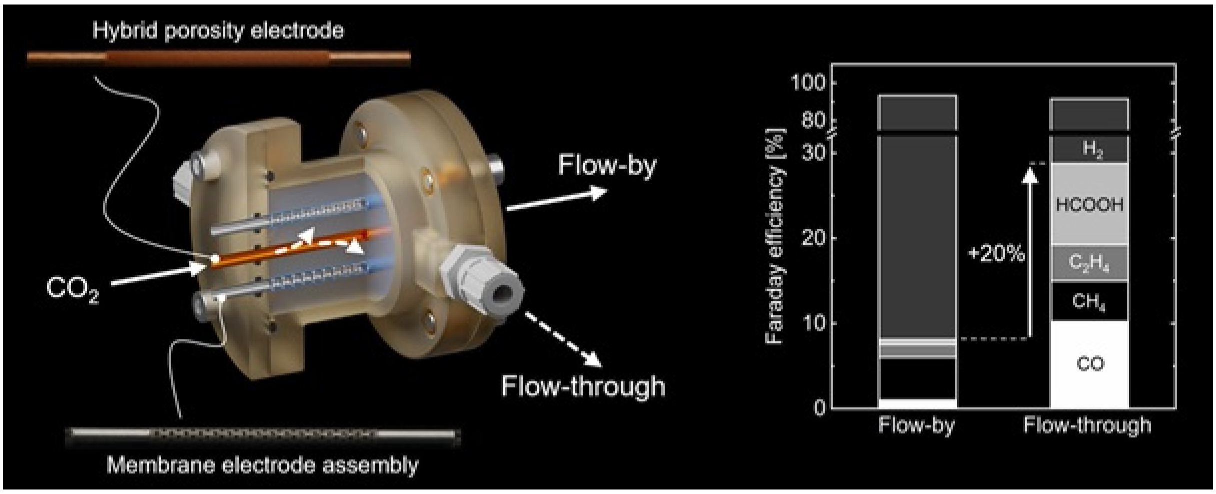

Figure 22: Flow reactor for 3D printed tubular gas diffusion electrode with tailored porosity.

Objectives

Integrated reactor systems contribute to concatenated reactions by i) housing different types of stimuli responsive catalysts and catalyst environment while ensuring efficient mass transfer ii) valorize multi-phase flow for efficient reactions and iii) integrated reaction and separation for intensified processes.

In FSC^2 we strive to design reactors, which facilitate stimuli responsive activation of catalysts and localized reaction control by leveraging advanced materials processing to trigger via electrical, thermal or pH-dependant actors. Additionally, we not only design reactors to cope with fluctuating input streams. We aim to dynamically control and pulse flow, temperature, wettability (and more) to optimize yields.

These entities will be self-optimized reactors, for which we employ model-based design and control strategies: Physically, the reactors will be equipped with online analytics but also visual observation to feed information into an ANN for real time control. In order to gain an understanding of the underlying physico-chemical effects, rigoros modeling will be applied. Surrogate models to cross length scales.

Work Program

The complexity of multiphase reaction systems results from the intricate interplay of different phenomena on micro-, meso-, and macroscale, rendering a significant challenge. Hence, there is a clear imperative to devise a systematic approach for the design, operation, optimization, and scaling of multiphase reaction systems. Within these systems, products are formed via bio-, chemo- or electrocatalysis, which can be intensified via ISPR. ISPR means separation of target molecules at their point of origin to suppress or minimise equilibrium limitations (Palkovits, Klankermayer, Leitner), product inhibition (Blank, Rother, Magnus, Lauterbach) and undesirable by-product formation (Wessling). This integrated approach improves operational efficiency and ensures optimal performance of multiphase reactors.

In microscale, the aim is to understand the reaction pathway by describing the principle trajectory of molecules from reactants to products. Further than defining the reaction stochiometrics, understanding involves fundamental knowledge of reaction equilibrium and kinetics, mass transfer, thermodynamic phase equilibrium, and fluid dynamics. For example, the mass transport of a single droplet, is recorded experimentally using a 2D Raman measurement cell and can then be modelled using spatially resolved discrete flow simulations (Pitsch). 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. Moreover, the concept of suspension electrodes may be extended to pickering emulsions, in which the second liquid phase enables ISPR or efficient reactant supply to the catalytic surface.

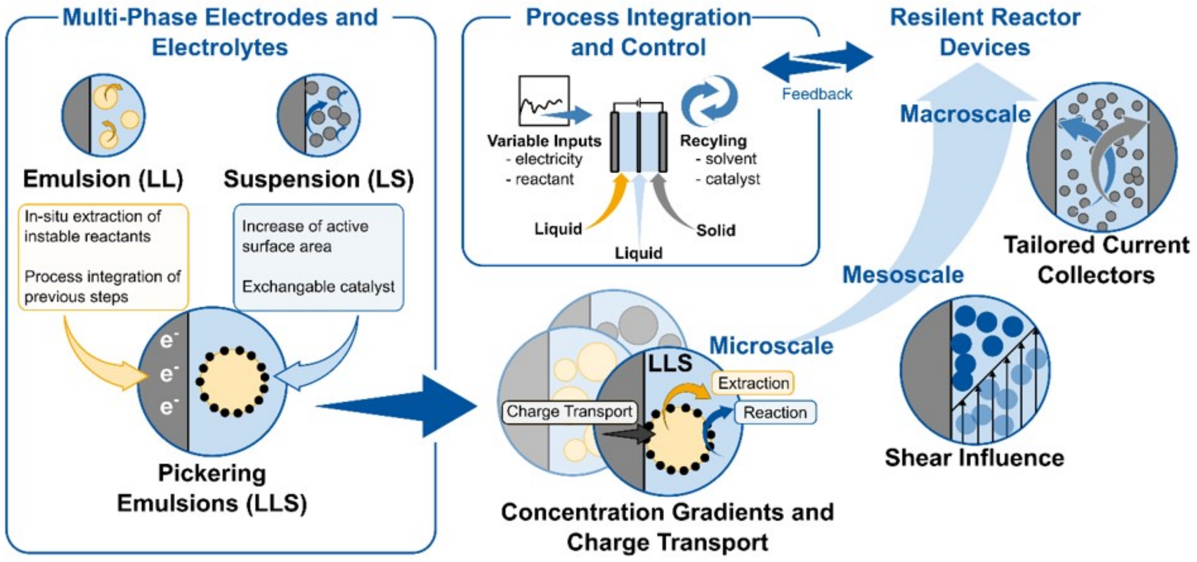

Figure AAA Scale based approach for multi-phase electrochemical systems.

Figure 23: Scale based approach for multi-phase electrochemical systems.

Figure 23 shows the multi-scale approach applied to electrochemical multi-phase reactors. Electrochemical interfaces and their reactions can be significantly enhanced by applying pulsed electrolysis. We will extend our computational approach with micro-kinetic modelling to experimental investigations elucidating the physicochemical phenomena at the interface. To derive crucial experimental data of such phenomena, measurements under relevant process conditions, which best approximate the operating space will be conducted using sophisticated analytic techniques, such as Raman spectroscopy, infrared spectroscopy, fluorescence life-time spectroscopy, distribution of relaxation times. Occurring phenomena need to be understood and interpreted in order to draw appropriate conclusions for process intensification in higher scales.

In mesoscale, our research methodology aims to derive a suitable model to couple previously measured microscale effects. For modeling, we use differential algebraic equations to dynamically model the complex parameter space of multiphase flow, reaction kinetics, mass transfer and thermodynamics which is experimentally not accessible in its quantity. In addition, we use hybrid modelling, integrating grey box models for numerical optimisation and real-time simulation to be able to handle contaminated and fluctuating feeds. Identification of physical phenomena sensitive to variations in substrate or power supply is critical to guide operational decisions to mitigate potential problems. To this end, the model framework is based on detailed and specifically recorded individual effects that are aggregated to a complex model of a multiphase reactor. On this basis, a pilot reactor will be equipped with sensors to enable performance and condition monitoring for status diagnosis and live parameterisation of data-driven elements. Therefore, specific equipment must be designed to meet the requirements of operation and control close to process conditions. For the electrochemical reactor with suspension electrodes, we strive to elucidate particle cluster formation and particle percolation in dependence of fluid flow conditions.

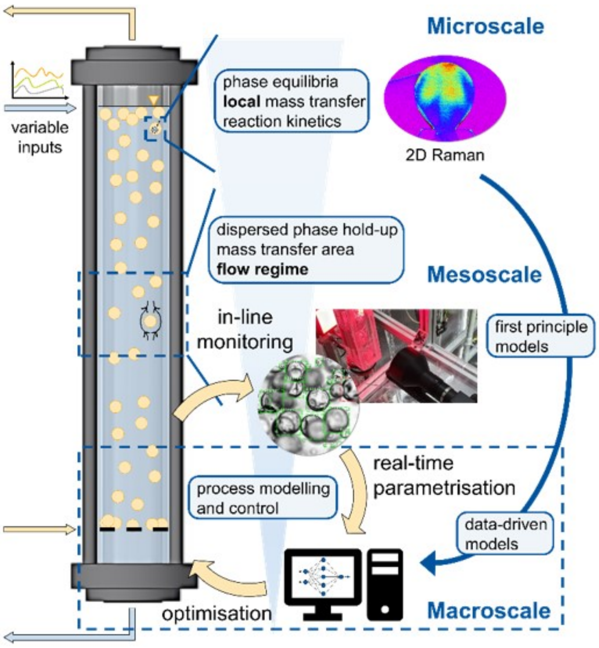

Figure 24: Autonomous and self-optimising multi-phase tubular reactor.

The learnings from operation and control in mesoscale will be essential for successful operation in macroscale. Complex thermodynamic and kinetic models can be replaced by surrogate and data-driven models that provide comparable accuracy with reduced computational effort and simulation time. Real-time simulation enables model predictive control, facilitating continuous optimisation of reactor behaviour based on dynamic data inputs. Computational sensitivity analysis helps to quantify the effects of fluctuations and variations in substrate and energy supply. We also focus on the development of in-line, on-line and at-line measurement techniques to obtain indicative quantities and facilitate on-line model parameterisation to ensure the reliability of our research results. The design of a dynamically and flexibly operable reactor should lead to an autonomous and self-optimising reactor control system, so that agile and adaptive operation can be realized.

4.5.3.4 Proposed Staff and Funding of SRA-CSP

Table 4.5.3.1: Proposed Staff in SRA-CSP

	2026	2027	2028	2029	2030	2031	2032
Staff category	**Number of persons**						
Professors	0	0	0	0	0	0	0
Independent junior research group leaders	0	0	0	0	0	0	0
Postdoctoral researchers	0	0	0	0	0	0	0
Doctoral researchers	21.5	21.5	21.5	21.5	21.5	21.5	21.5
Other staff	0	0	0	0	0	0	0

Table 4.5.3.2: Funding Request for SRA-CSP

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff (Total for 4.5.3)	1638	1687	1738	1790	1844	1899	1956
Direct project costs (excluding staff)	300	420	262	230	215	215	215
Total instrumentation < €150,000	360	355	0	0	0	0	0
Total instrumentation > €150,000	180	0	0	0	0	0	0
DASbox® Mini Bioreactor System	180						

Instrumentation below 150 000 €

The Data-driven development of homogeneous catalysts for reduction reactions require a high-pressure equipment with adapted analytics (125 k€). To analyze phase equilibria and compositions of mixtures with little experimental effort, a high-pressure differential scanning calorimetry has to be procured (120 k€). For obtaining highly accurate density measurements of liquids over a wide range of temperatures and pressures, a high-pressure density meter (50 k€) is required. To gather important thermodynamic fluid data through small sampling procedures by not only maximizing the data collection through optimal experimental design but also minimizing the used resource, a 3-phase tailor-made measuring cell (60 k€) shall be procured. A multi-fold parallel pressure reactor is required to develop a flexible catalyst platform for single site and single atom materials (120 k€). To study electrocatalytic transformations, an online Benchtop nuclear magnetic resonance (NMR) spectrometer for analysis has to be procured (50 k€). To perform *in-situ* product analysis during the gas fermentation, a NMR benchtop spectrometer is required (90 k€). For the evaluation of biochemical pathways to synthetic biofuels, 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 2x DASbox Mini Bioreactor System is required (360 k€).

4.5.4 Strategic Research Area: Translational Catalytic Processes

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

Add short summary of SRA here

In the development of new concatenated synthetic pathways, there is a strong focus on developing novel transformations and their interconnection. This requires in many cases screening and testing of catalytic activity and selectivity as basic performance criteria using model compounds or prototypical substrates. The translation into actual catalytic processes requires additional fulfilment of robustness and stability considering the complexity feedstocks, their quality variation, and the integration of their supply with the catalytic conversion (Figure 25). Feedstock complexity is particularly challenging for bio-based raw materials and substrates that are often mixtures or even composite materials. Integration of supply and conversion is a major target for CO_2-based processes ranging from CCU concepts to direct air capture coupled with catalytic transformations. 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. 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 chemical pathways to processes in this Strategic Research Area (SRA) thus covers the technology maturity progression, from laboratory experiments with model substances to interlinked unit operations comprising upstream feedstock supply and advanced energy input technologies.

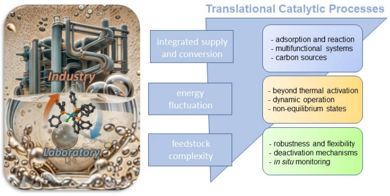

Figure 25: ?

Strategy and Structure of SRA

The research in the SRA focuses on the impact of feedstock complexity (Sub-Topic 1) as well as dynamic operation due to energy fluctuation and feedstock variation (Sub-Topic 2) on the robustness of catalytic processes. In particular, the challenges and opportunities arising from these issues are addressed in the context of concatenated pathways and integrated process concepts (Sub-Topic 3). The overall transformations under scrutiny are defined either from the progress in the area Concatenated Synthetic Pathways (4.5.X) 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.

The leading role of Principal Investigators (PIs) from The Integrated Fuel & Chemical Science Center (FSC^2) in industrial-academic consortia (Kopernikus, Carbon2Chem, ETOS, Bio4MatPro, AUFBRUCH) and strategic collaborations (CAT Catalytic Center, BioSC) provides detailed insight into the challenges associated with real-world feedstocks including composition, impurities, and availability. This information provides a unique information basis to design and plan the methodological approaches in fundamental science of the cluster accordingly. In selected cases, this specific network offers access to actual feedstocks to validate the progress within actual industrial environments.

Objectives:

- Fundamental understanding of the impact of multi-component mixtures or impurities in feedstocks on catalyst activation and de-activation processes and strategies to overcome potential negative interferences.
- Design of variable and adaptive catalytic systems to deal with energy fluctuation and feedstock variability and their demonstration for relevant transformations.
- Novel concepts for integration of feedstock supply and catalytic conversion and their validation and evaluation for energy savings and carbon efficiency.

4.5.4.1 Feedstock Complexity and Variation

Blank

Add short summary here. Based on previous experience, FSC^2 develops a broad methodological portfolio on the chemical deconstruction of the major components in lignocellulose and related polymeric structures to provide bio(hybrid)fuels and platform chemicals (e.g., carbohydrates, furanics, monomers), together with a strong competence in catalytic CO_2 conversion. Understanding and overcoming the challenges of feedstock complexity, including gases, impurities, variations in composition on different time scales, and the use of carbon source mixtures (e.g., biomass + CO_2), will be the focus of the research in FSC^2 . The incorporation of nitrogen-containing building blocks opens an additional dimension of complexity for chemo-, bio- and electro-chemical processes.

Previous work

A common strategy does deal with the presence of potential inhibitors is the development of low-cost and low-energy steps for their removal to protect the bio- or chemo-catalyst from deactivation. For example, the diamine TDA present in polyurethane hydrolysates from polymer-recycling was identified as major inhibitor with toxic effects on engineered microbes developed in The Fuel Science Center (FSC). It was shown that TDA could be removed from the monomer mixture by reactive extraction allowing successful conversion of the resulting PU hydrolysate by an engineered microbial consortium to rhamnolipids ([154]). A specific microbe could be engineered to produce 3-(3-hydroxyalkanoyloxy)alkanoic acid (3-(3-hydroxyalkanoyloxy)alkanoic acids (HAAs), [155]) as platform intermediate for chemo-catalytic or electrocatalytic [156] 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 [157].

Selective adsorption is also a possibility to reduce the complexity of alternative carbon sources. The simple fractionation of fructose from a glucose-fructose mixture by tailoring cross-linked boronic acid polymers after biomass hydrolysis is such an example [158]. Notably, polymer adsorption proved more generally viable and allowed simple process setups, while guaranteeing high selectivity by engineered molecular structures. Functional phenylboronate polymers were used for the recovery of biogenic diols from aqueous media [159]. For example, 2,3 butanediol was recovered by this technology from microbial fermentation broth [125]. Notably, diols can also exhibit product inhibition or hinder further conversions acting as poisons for whole cell transformations. The successful application of the polymer adsorption for efficient integrated product removal was demonstrated for production of itaconate by an engineered smut fungus ([160, 161, 162, 163]).

Recently, we could showcase that CO_2-derived substrates such as formate and acetate can be metabolized by smut fungi, [92] increasing upon co-feeding significantly the yield of itaconate from glucose. Using CO_2-derived weak organic acids as carbon source for microbes opens novel opportunities for biohybrid production, but requires to decouple their acidity from the proton gradient of microbes by strain and bioprocess engineering [140, 164]. In the FSC, the synthesis of formate and acetate from CO_2 was studied extensively [165, 88, 68, 71]. Notably, the products of these reactions might well be suited as substrate for biotechnology even if selectivity is not perfect, because side products such as formaldehyde or methanol are readily detoxified by the microbes or ideally used as energy source. On a systems level, the CO_2 point sources should be envisaged to be also part of the bioeconomy to maximise “de-fossilization” on a systems level.

Indeed, 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 CO_2 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 active under 110 bar of hydrogen pressure and the organometallic catalyst was separated from the fermentation broth in an organic/aqueous biphasic system ([134], Figure 26).

The research of FSC has demonstrated the beneficial effects of long chains alcohols as components in Fischer-Tropsch-based fuels (HyFiT fuels, see chapter XXX). 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 with very high turnover numbers and selectivities. Observation

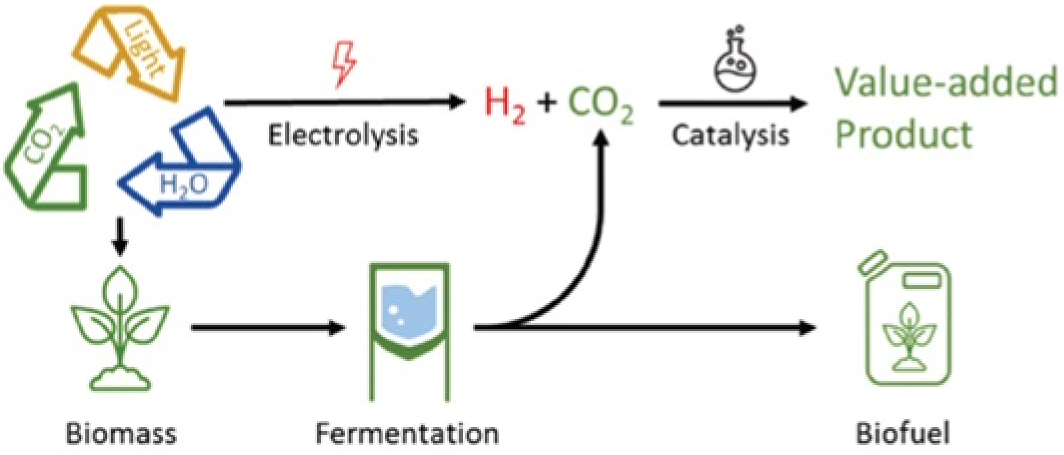

Figure 26: Utilization of renewable resources for biofuel production through fermentation and additional catalytic CO2-reduction to value-added products. [134]

using a borescope under operando conditions using a specifically designed high pressure reactor was crucial for the understanding of the complex phase behaviour ([166, 167]).

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 CO_2 conversion proved remarkably robust allowing depolymerisation even for end-user products to provide useful platform chemicals [168]. This provides access to another important source of carbon within the systems boundaries of a de-fossilized value chain [82, 169].

In addition to the carbon source, also the “green” hydrogen may show different impurities or by-products depending on its production. While traces of oxygen or water may be contained in H_2 from electrolysis, CO or CO_2 can be present in H_2 obtained from biomass reforming. We have demonstrated that the selectivity for hydrogenation of biomass-derived substrates over certain heterogeneous catalysts depends critically on the use of pure H_2 or H_2/CO_2 mixtures [170]. For example, furfuralacetone is hydrogenated either to the fully saturated alcohol under H_2 or the partially saturated ketone under H_2/CO_2 with high selectivity (Figure XYZ). The effect was found to be fully reversible and quite general [171] resulting in adaptive control of product formation depending on the absence or presence of CO_2. *In situ* spectroscopic techniques revealed the reversible formation of surface-bound formate species as molecular reason for the drastic change in performance.

In summary, FSC^2 can build on a large body of experience to study the effects of complex feedstocks on individual catalytic steps and in particular also 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.

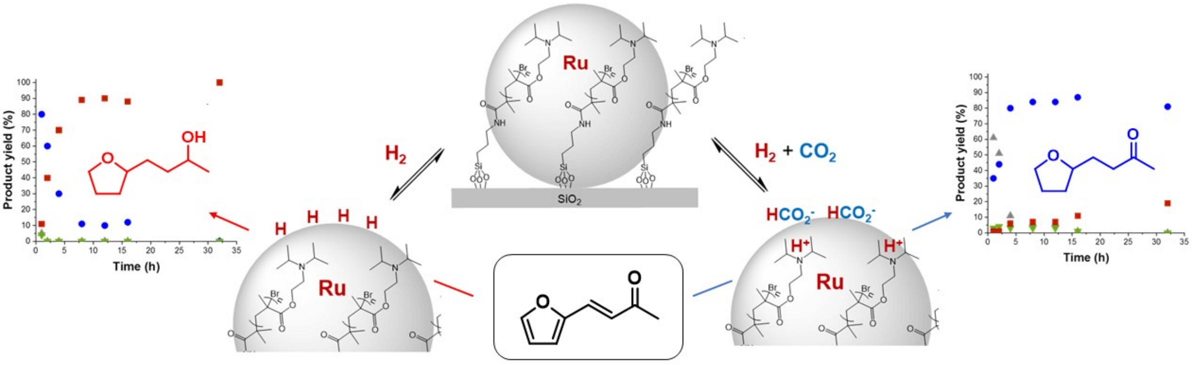

Figure 27: Adaptive catalysis produces either the fully saturated alcohol or the partially saturated ketone from bio-based furfuralacteone depending on the use of pure H_2 or H_2 in presence of CO_2. [170]

Objectives

- Rational development of robust and flexible (“adaptive”) catalytic systems that are able to cope with the complexity (composition and variation) of renewable feedstocks
- Fundamental understanding of the influence of raw material complexity on catalyst, transformation, and reaction system
- Experimental and computational techniques to study the dynamics of such catalytic systems across time and length scales

Work Program

The fundamental basis for the development of catalytic systems capable of coping with feedstock complexity requires a detailed understanding of the interaction of the catalytic system with not only the reagents, but also 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 with the catalysis teams on basis of relevant FSC^2 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 experiment methods will be applied for planning and mathematical 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 machine-learning approaches will be advanced towards predictive potential (Mitsos, Pitsch, Kethan, Leonhard).

The relevant FSC^2 reaction systems will build on its previous success representing a major line of research on feedstock complexity in the context of catalytic production of “biohybrid” molecules while expanding this area towards targets from the chemical value chain. Recent review articles highlight the approaches taken with FSC and outline current trends and future developments [172, 173]. EXAMPLES

Capitalizing on the very successful integration during the last phase of electrocatalysis and electrosynthesis in the technology toolbox (see section 4.5.2.2 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 FSC^2 is the coupling of biocatalytic acetoin formation with electrocatalytic oxidation to butanone, it was able to overcome the problem that the electrocatalysis in cultivation broth suffered from parasitic reactions due to dissolved media components [146]. The analytical platform provided by the Mayrhofer group allows specific insights into molecular interactions at the electrode materials particularly relevant for CO_2-based processes [174]. The newly acquired experience of the Waldvogel team with scalable electrosynthetic methods utilizing technical grade feedstocks will be highly beneficial in this context [175].

Reflecting the increasing importance of “green ammonia” at the interface of energy and chemistry (see section??), FSC^2 will strategically extend its efforts on catalytic synthesis and processes towards nitrogen-containing building blocks and products. For biomass synthesis, the rule of thumb is $CH_{1.8}O_{0.5}N_{0.2}$. Hence, for every five mol of carbon one mol of nitrogen is required. While the absolute tonnage of ammonia and it’s salts is small compared to the fertilizer market, the required amount of N will increase dramatically when developing increasingly microbial production processes or concatenated processes, as outlined above. Again, FSC^2 is in a unique position to address the challenges resulting from integrating renewable N-sources via ammonia into biotechnological processes and to evaluate competing demands (fertilizer, hydrogen carrier, fuel, feedstock for biotech) on a systems level. Recent research demonstrates the potential to combine biobased feedstocks, syngas, and amines for the construction of nitrogen-based intermediates and products [176] opening promising development lines for future FSC^2 research. Promising approaches to activation of ammonia and ammonia-derived building blocks include chemo-catalytic as well as electro-catalytic processing options [177, 178, 179].

In summary, the complexity of renewable feedstocks will be researched including the effects of mixtures, quality variations, and impurities. This reaches beyond carbon molecules as outlined above for the quality of hydrogen or the exploitation of ammonia and nitrogen-based building blocks. Obviously, the integration with the energy input is of major importance and the implications of the panned FSC^2 research on energy integration and fluctuation is explained in the following section.

Leitner

4.5.4.2 Energy Input and Fluctuation

Add short summary here.

With electricity from renewable resources becoming the main energy source for chemical processes, novel opportunities arise to control catalytic transformations on a molecular and process level. In particular, concepts can 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 [180]. While mechano- and photochemical activation will continue to be considered, the cluster research in this area will focus mainly on electrocatalysis and magnetically induced catalysis.

Previous work

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 CO_2 can be conducted very effectively under ball milling conditions[181]. The potential of solid-state NMR to obtain fundamental insights into mechanochemical processes has been demonstrated and critically discussed[182]. The technique will be further developed in the early stage of the next phase to ensure its availability in the pool of methods accessible to FSC^2[182]. (Bolm; Wiegand)

Electrochemical approaches to drive CO_2 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 at Max Planck Institute for Chemical Energy Conversion (MPI CEC).

The combination of proton reduction in water splitting to generate hydrogen with concomitant organic reactions utilizing the anodic oxidation potential is viewed as attractive relay between energy and chemical conversion [101]. WALDVOGEL TO BE ADDED Conducting electrocatalytic reduction of hydrophobic substrates has been achieved in using pickering emulsions using catalytically active surfactants based on Pd-decorated carbon nanotubes.

In a FSC^2-typical collaboration between biotechnology and electrocatalysis, the fermentation of carbohydrates to acetoin has been coupled directly with its electrochemical de-oxygenation to 2-butanone, a potential fuel component[146].

?[183]

Magnetic induction provides an effective tool for very localised heating reacting instantly to dynamic changes in the power supply. Research within FSC has demonstrated the possibility to decorate traditional and even commercially available heterogeneous catalysts with magnetically responsive nanoparticles [184]. Due to very high specific absorption rates (SARs) under alternating magnetic fields, iron carbide nanoparticles (ICNPs) were shown to allow catalytic hydrogenation and hydrogenolysis under significantly lower bulk temperatures due to local hot spot formation as well as real-time on/off switching of the catalytic activity. The revers catalyst design to use the ICNPs as support for active metal nanoparticles has also been established

[185].

Objectives

- Design and demonstration of catalytic processes based on alternative methods for energy input (electro-, mechano, and magnetic activation)
- Evaluation of these methods for flexible and adaptive response to fluctuations in primary energy supply
- Fundamental understanding of activation and de-activation processes within the catalytic system on molecular level and across material interfaces.

Work Program

Future work on electrochemical approaches for CO_2 conversion will focus on advanced materials and cell designs (Mayrhofer, Palkovits, Waldvogel, Wessling). In particular, the intricate interplay of the catalytic transformation with the transport phenomena at the material interphases will be studied under dynamic operation conditions [Adv. Sustainable Syst. 2023, 7, 2300077]. The coupling of reductive and oxidative processes to maximise energy and carbon efficiency will be addressed systematically [ACS Sustainable Chem. Eng. 2023, 11, 18, 6822–6828]. Innovative reactor design will pay a crucial role in this endeavour [Electrochemistry Communications 150 (2023) 107477].
MATERIALS –> REGINA
[182]

Palkovits

4.5.4.3 Integrated Feedstock Supply and Conversion

Add short summary here.
Based on a fundamental understanding of the influence of raw material complexity on catalyst, transformation and reaction system, 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 CO_2 an integrated supply, separation and conversion can be envisaged valorising bio-, chemo- or electrocatalytic transformations.

Previous work

Within the diverse feedstock base, carbon dioxide poses specific challenges. It can be provided in pure form by direct air capture (DAC) associated with high energy demands. Alternatively, CO_2 is available in form of carbonate or amine solutions from scrubbing processes or even as (highly) diluted and multi-compound feedstock 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 regarding accompanying substances, concentration and purity. Environmental merit order curves were developed to rank CO_2 sources according to their environmental impact over the available CO_2 supply to identify favorable locations for CO_2 utilization with lowest environmental impacts, so-called CO_2 oases (von der Aßen).[186, 187][x]

To enhance efficiency of carbon capture, advance in tailored absorbents, adsorbents as well as process design were targeted. Therein, tailored adsorbents bear the potential to significantly reduce the energy demand of DAC. Previous studies highlight the potential of N-containing carbons enabling high capacity and selectivity, respectively. Material morphology and surface functionality were identified as major design criteria. For covalent triazine frameworks (CTF) derived by trimerization of dinitriles, the influence of framework composition and materials' temperature treatment was demonstrated. With CO_2 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 CTFs (Figure 28) [188].

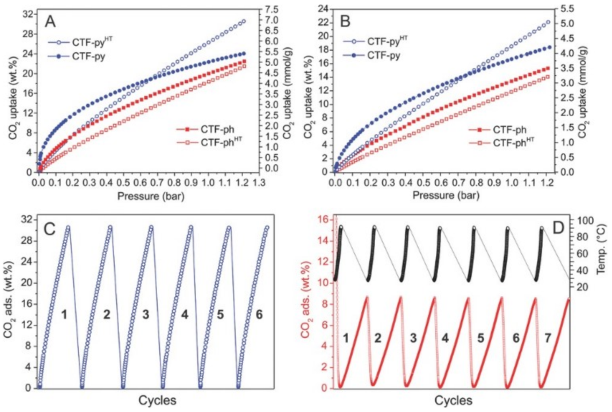

Figure 28: CO2 sorption cycles at T = 273 K on a high temperature treated pyridine-based CTF confirming high stability. [188]

Also, polyacrylonitrile-based carbon nanofibers (CNFs), prepared at different carbonization temperatures, showed promising properties for CO_2 sorption [x,y]. The best performance was found for the CNFs prepared at 600°C with measured CO_2/N_2 selectivity of up to 194 (Figure 29) [189].

In contrast to packed beds for adsorption processes, hollow fiber, or tubular, adsorption devices enable controlled flow conditions, low pressure drop and facile scale-up via numbering up. carbon nanotubes (CNT)-based microtubes were impregnated with polyethylenimine and employed for temperature swing adsorption of CO_2 [190]. A module with multiple tubes in parallel enabled scale-up, and load-flexible operation [191]. Overcoming the need for thermal energy for desorption, the tubular adsorbers were adapted allowing direct Joule heating of silicon carbide or zeolite enforced fibers [192].

Integrated carbon capture and conversion presents a promising alternative to the sequential CO_2 capture, storage and release of CO_2 followed by its conversion. As a first step, direct hydrogenation of CO_2 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 [78]. Also, along the value chain of high temperature co-electrolysis of CO_2 and water to CO and H_2 followed by CO_2 hydrogenation, direct integration could be demonstrated

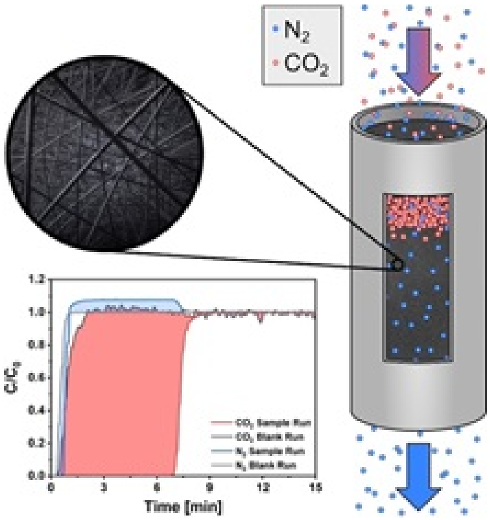

Figure 29: Breakthrough curves. Adsorption was performed with 50 % He, 45 % N_2, and 5 % CO_2 at 273 K and 5 bar on PAN-based CNFs carbonized at 700°C and is shown in comparison to a blank run. [189]

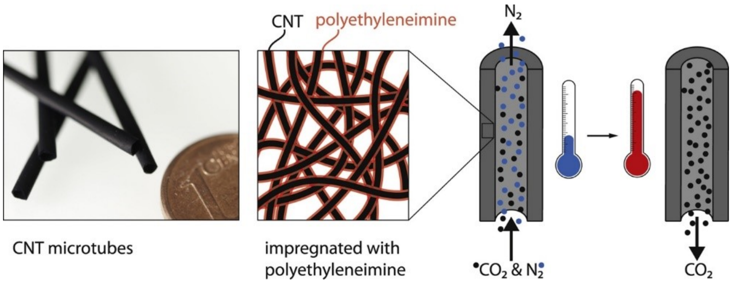

Figure 30: ?

[193]. Especially the water content of the feed from co-electrolysis proved crucial for catalyst activity and stability. While a commercial Ni/Al_2O_3 catalyst showed fast activity loss for water contents exceeding 10 %, a tailored NiFe/(Mg,Al)Ox system could even operate at 30 % water content and was readily regenerated by calcination.

In the thermo-catalytic hydrogenation of CO_2 to produce carboxylic acids, activity and selectivity could be significantly enhanced by supplementing the primary liquid decane reaction by a second liquid product conservation phase (methanol) allowing continuous extraction by an acid-amine complex [194, 195]. Another two-phase system [134] 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 [4]. It was applied to develop in situ purification processes particularly for microbially produced carboxylic acids [196, 197, 198].

not used text Beyond CO_2, also the selective separation of biomass-based intermediates such as sugars, carboxylic acids, amino acids and diols[199, 200] from complex mixtures has been demonstrated enabling novel integrated processing strategies along the value chain. In a case study on itaconic acid, selective separation from crude fermentation broth is possible with novel adsorbent systems [lit Palkovits]. However, electrocatalytic studies have highlighted the possibility to directly convert biotechnologically derived platform chemicals such as itaconic acid or HAAs without any prior separation [examples itaconic acid Palkovits, HAAs Blank Pischinger Palkovits].

Objectives

- Enabling tools and design criteria for an integrated separation and catalytic transformation of CO_2 feed streams.
- Fundamental understanding of trade-offs in valorising real feedstocks by intensified process concepts compared to sequential separation and conversion.
- Identifying the potential of dynamically operated.

Work Program

The purification and compression of CO_2 prior to a reduction reaction are both energy-intensive steps. The integrated carbon capture and conversion (ICCC) promises more energy-efficient processes. In an ICCC process, the provision of a highly concentrated CO_2 gas phase is omitted by directly converting the sorbent-bound CO_2, instead of releasing it into a gas phase. The degree of integration of both process steps can vary strongly. Thus, we aim to address the subject of 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) CO_2 thus may allow bringing CO_2 capture and conversion together (Leitner).

On the molecular level, orthogonal material design will enable integrating tailored sorption sites and catalytically active centers for valorising 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. ...Understanding necessary molecular proximity

Absorption systems for CO_2 are often of aqueous nature (MEA, alkaline scrubbing etc.) fostering the dissociation to H_2CO_3, $HCO_3{}^-$ and $CO_3{}^{2-}$. Inherent to the processing of this system is a meticulous observation and control of pH. Implementing an electrochemical production of H^+ and OH^- ions will enable generating the driving force necessary to couple alkaline scrubbing and CO_2 conversion. Two potential conversion pathways are going to be investigated in this regard: thermo-catalytic bicarbonate conversion and bicarbonate electrolysis.

In the first pathway, alkaline scrubbing is used to separate CO_2 from flue gas or air (DAC) leading to the formation of bicarbonate/carbonate. Instead of reversing this process to obtain a concentrated CO_2 stream, feeding the bicarbonate/carbonate salt directly to catalytic CO_2 activation will be targeted avoiding an energy-intensive CO_2 compression step. A novel ICCC process has been developed based on recent research on heterogeneously catalyzed formic acid production from bicarbonate/carbonate in aqueous solution. To couple capture and conversion, the acid and base need to be generated electrochemically. Whereas the base regenerates the absorption capacity of the alkaline scrubbing unit, the acid protonates the carboxylic acid produced in the CO_2 conversion step. Several fundamental challenges need to be addressed. First, the catalytic system of the reactor must be adapted to a bicarbonate/carbonate feedstock and improved with respect to efficiency and productivity. Opposed to the thermo-catalytic approach suggested in the literature, a bio-catalytic conversion will also be considered. Second, the complex interactions between the bicarbonate/carbonate provision, the hydrogenation reaction system, and the hydrogen supply must be aligned to operate the conversion unit. Third, an electrolyte composition must be identified that fits the requirements of the CO_2 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 CO_2, 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 CO_2 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 integration of CO_2 absorption and conversion unit, as it has been shown that the CO_2 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.

On the system level, the methodological concepts are mirrored in dynamic modelling of material behavior and life-cycle assessment (LCA) for Designing Sustainable Integrated Carbon Capture and Conversion Processes in Volatile Energy Systems (van der Aßen). The role of Combining Single reactor avoids CO2 transport and enables heat integration between the CO2 capture and conversion steps.

4.5.4.4 Proposed Staff and Funding of SRA-TCP

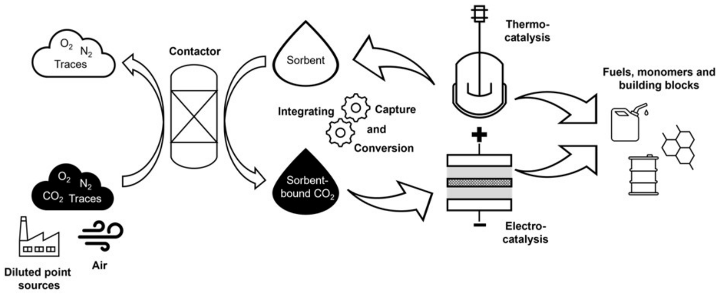

Figure 31: Integrated capture and thermo-catalytic or electro-catalytic conversion of sorbent-bound CO_2 to fuels, monomers and building blocks.

Table 4.5.4.1: Proposed Staff in SRA-TCP

	2026	2027	2028	2029	2030	2031	2032
Staff category			**Number of persons**				
Professors	0	0	0	0	0	0	0
Independent junior research group leaders	0	0	0	0	0	0	0
Postdoctoral researchers	1	1	1	1	1	1	1
Doctoral researchers	15.5	15.5	15.5	15.5	15.5	15.5	15.5
Other staff							

Table 4.5.4.2: Funding Request for SRA-TCP

	2026	2027	2028	2029	2030	2031	2032
Funding category		**Totals per year in thousand euros**					
Staff (Total for 4.5.4)	1181	1216	1253	1291	1329	1369	1410
Direct project costs (excluding staff)	205	285	185	185	185	185	185
Total instrumentation < €150,000	375	130	60	0	0	0	0
Total instrumentation > €150,000	160	150	0	0	0	0	0
DASbox® Mini Bioreactor System	160						
Online analytics suited for high temperature reaction systems (e.g. NMR, GC)		150					

Instrumentation below 150 000 €

For the investigation of ordering phenomena and molecular interactions in immobilized catalysts by solid-state nuclear magnetic resonance (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 infrared (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 microwave (MW)-enabled ICCU, 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 (160 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 (150 k€).

4.5.5 Strategic Research Area: Resilient & Adaptive Conversion Systems

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 as well as 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 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 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 this SRA 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.

The results of RACS are fed back to the other SRA consistently to enable an iterative research process within FSC^2 based on an ex-ante evaluation of developed process paths and fuels.

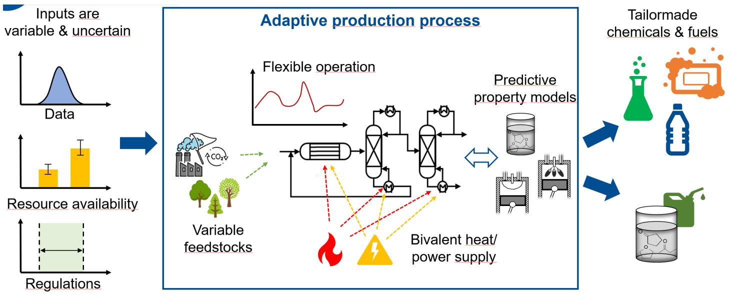

Figure 32: Rough draft of fuel design for resilience and adaptivity

Mitsos

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 design forum CROSSREFERENCE, the research is tightly integrated with the whole FSC.

Previous work

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., [10.1016/j. compchemeng.2019.106712,10.1002/cssc.202101704]. Moreover, we have been very active at the intersection of energy and chemical processes, e.g., [10.1016/j. compchemeng.2023.108582]. 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., [10.1016/j. compchemeng.2020.106890,10.1002/aic.10456].

Incorporating adaptivity and resilience onto chemical & fuel design will result in numerically very challenging optimization problems. 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 [10.1002/aic.16986,10.52202/069564-0223]. The resulting optimization problems fall in the class of robust nonlinear programs for which we have best of-a-kind algorithms [10.1007/s109 57-021-01813-2] and have released open-source optimization tools [`https://optimization-online.org/?p=24914`] 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 [10.1007/s12532-021-00204-y].

Objectives

- Overcome the limit of current production processes which exhibit insufficient flexibility to cope with volatility of renewable energy and feedstocks and in economic boundary conditions.
- Extend the fuel design methodology to new boundary conditions, e.g., drop-in fuels for ship combustion engines and fuel cell-based propulsion.
- Identify critical green chemicals to enhance the resilience and adaptivity of fuel, energy, and chemical systems despite extreme uncertainties.
- Account for novel unit operations in process operation: intensification and electrochemistry

Work Program

The fuel and chemical design is at the core of The Fuel Science Center (FSC). 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. 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, see also the next subsection (“System integration”) using coupled supply chain, process, and combustion models.

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. In particular, we emphasize optimization-based identification of drop-in fuel including oxygenated blending components and production process including integrated carbon capture and conversion. 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 CROSSREFERENCE, such as direct liquid fuel cells. 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 predictive fuel blend property models for material compatibility, toxicity, and emission formation. 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. 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.

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. 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

Overall, the desired tasks result in very challening mathematical formulations. We plan to utilize data-driven surrogate models, based on machine learning concepts, to overcome computational expense. 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

Walther

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 of FSC^2, and extend the system boundary towards competitive 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.

Previous work

The target of Competence Area 3 (CA3) in FSC was to develop a system-wide design perspective to guide and evaluate novel transformation pathways for the transformation towards flexible value chains for bio-hybrid fuels. An interdisciplinary team of researchers from biology, engineering, economy, and social sciences developed an integrated framework assessing and optimizing the sustainable and cross-sectorial value chains, integrating techno-economic, sustainability, and social aspects, as well as policy implications.

Research in FSC analyzed conditions for market adoption and diffusion of bio-hybrid fuel value chains. Combined micro- and macro-level analyses ([201]) 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. Analyzing supply chain stages and their interlinkages in detail, results showed how short- and long-term availability of feedstocks determines technology choice and structure of supply chains ([202, 203, 204]AmiriZenodo24). (Meta-)analyses provided predicted future demand of fuels for different scenarios ([205]). Prospective fuel candidates were determined regarding market diffusion barriers and sustainability factors with a possibility-based multi-criteria approach ([201, 206]Hendiani24).

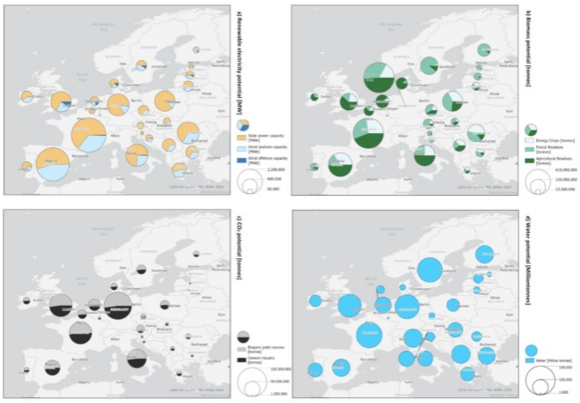

Figure 33: Potential of resources in EU countries a)Renewable electricity potential b)Biomass potential c)CO2 potential d)Water potential [203]

Public perception was analyzed FSC as multi-faceted perspective of risks and benefits of fuel products, production processes and infrastructural changes [207, 208, 209, 210, 211]based on a multi-stage iterative empirical methodology [212, 213, 214]. Research revealed risk perception of fuels as a complex construct, segmented into distinct domains such as health, environment, and technical risks (Figure xx), and influenced by cognitive and affective components [215] and individual factors [216]. A positive perception of alternative fuels [217, 209] requires comfort and affordability as well as environmental and toxicity benefits of fuels along with infrastructural developments and political communication [218, 217, 219, 220, 221]. 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 [222, 223, 224, 225, 226]. For policy analysis, a comprehensive policy review of European, national, and regional policies across multiple scales and sectors was carried out (Torkayesh1f). Research 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 [206](Torkayesh1d, Torkayesh1e,). Also, the techno-economic and social perspectives are only insufficiently considered compared to the environmental perspective (Torkayesh1d). 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 [227]. The above-mentioned aspects were integrated to design optimal fuel supply chains by prescriptive optimization herein accounting for long-term transformation, feedstock variability, import scenarios, and high integration of the fuel and energy sector. Sector-integration was regarded by model extension. On the one hand, 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 [229, 230, 204, 231]. Myopic solution approaches proved appropriate as they reducing the computation time drastically while still providing adequate objective values [204]. On the other hand, value chain mod-

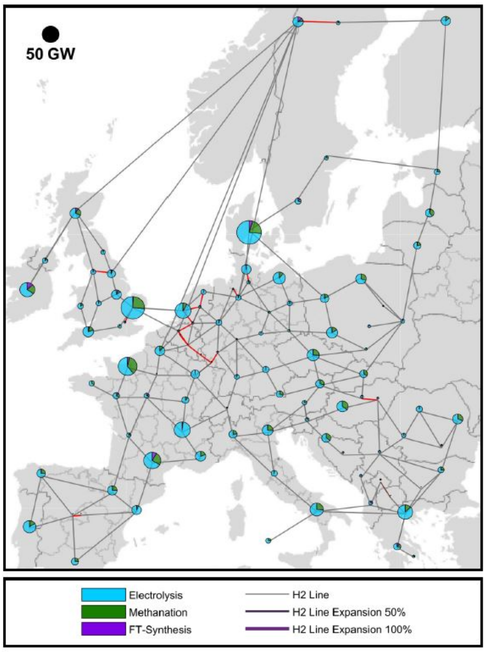

Figure 34: Potential Distribution of Power-2-X Plants in 2050 [228]

els were extended to integrate 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 decomposition [202]. Models were then applied to real-world case studies. 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 [228]. Model extensions explored the trade-offs between cost, land-use, and water-use [203], the consideration of policy requirements [232, 233]Zardoshti;, and the innovative integrating of social acceptance in the optimization-based design of bio-hybrid fuel supply chains via multi-objective optimization [234, 211]. 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 [235].

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 is innovative as it enhances the FSC approaches by:

1. extending 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 regard for the global perspective of value chains.
2. establishing a systemic risk assessment framework by quantifying and evaluating the impact and interrelations of endogenous and exogenous transformative and operational risks.

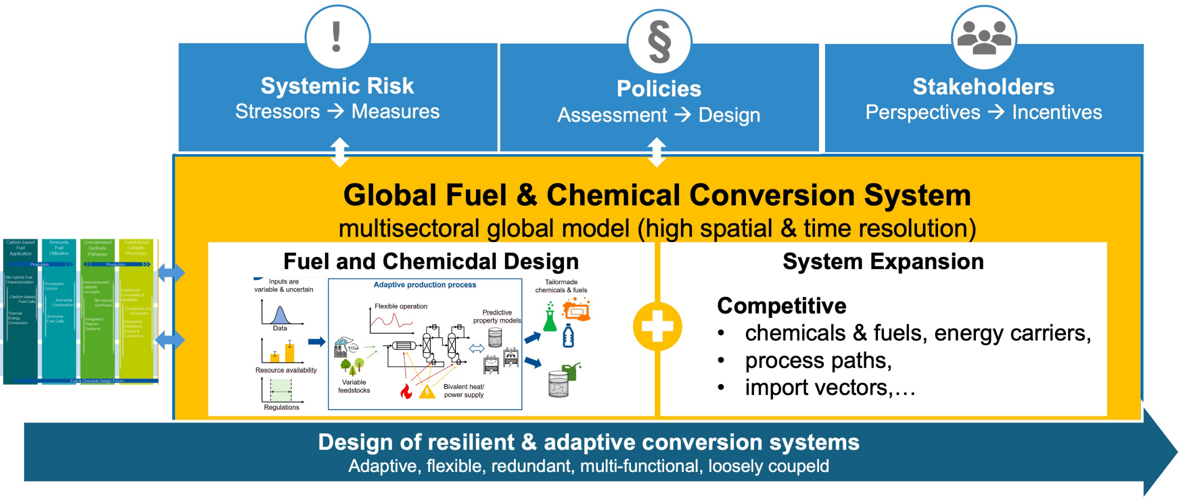

Figure 35: Design of resilient and adaptive conversion systems by integration of stakeholders' incentives, policy design, and systemic risk measures

3. developing a predictive agent-based approach that is explicitly regarding stakeholders' perspectives and their influence on the overall system's level and vice versa,
4. developing a prescriptive policy design that 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 of FSC^2 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), and the conclusive model for the design of 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 risks that go along with the installation of global renewable fuel and chemical conversion systems (e.g., [236]). FSC^2 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 (*Arning, Ziefle*) deriving risk perception dimensions (e.g., financial or environmental risks), 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. 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 [237, 238, 239, 240]Arning/Venghaus. Thus, we overcome the centralized perspective that omits stakeholder-specific decisions (e.g., [241, 242, 243], and analyse stakeholders' roles and positions in the value chain, objectives, constraints, perceptions, and risks using social empirical research, (social) network analysis, data mining, and machine learning (ML) (*Walther, Venghaus, supported by Arning*). This allows to derive stakeholder-specific decision models. The behavior and interrelations between stakeholders are then 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 can 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. The system has to 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 effects, feedback loops, and delays among system's components with a System Dynamics 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

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To enable FSC vision of "near-to-zero environmental impacts", we assess the environmental impacts of fuels and chemicals with the life-cycle assessment (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 holistically, reliably and on a broader scope. Based on the LCA methodology, we aim to develop a Sustainability Assessment for future fuels & chemicals. We advance LCA for an 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

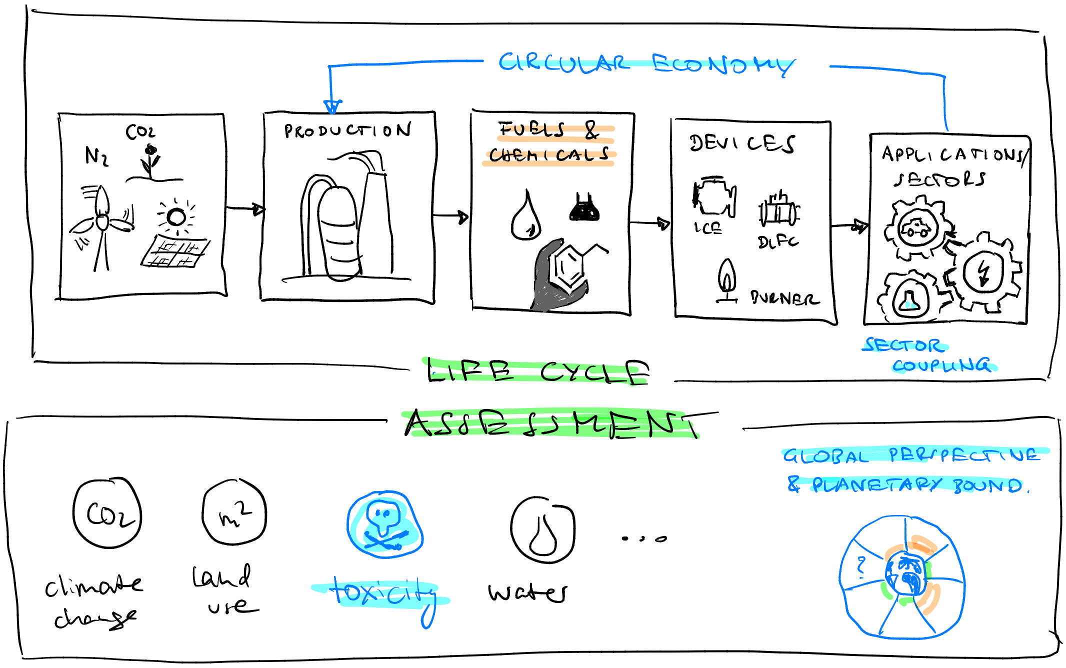

Figure 36: The Sustainability Assessment will cover the entire life-cycle of fuels & chemicals. Methodological extensions are highlighted in blue: toxicity prediction, sector-coupling, planetary boundaries (incl. socio-economic impacts) and circular economy.Figure needs to be updated and 'professionalized'

conversion systems, e.g., ammonia synthesis, integrated CO_2 capture and conversion, and direct-liquid fuel cells. A small and frequent feedback loop with researchers from the other Strategic Research Areas (SRAs) will guarantee that technologies are developed not only for efficiency, resilience and adaptability, but also for maximum sustainability.

Previous work

The LCA methodology has already been successfully applied and extended in FSC as well as in individual projects by the (new) Principal Investigators (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 an LCA study [23].
Major gaps in toxicity assessment of fuels & chemicals within LCA are the lack of toxicity data, the assessment of mixture toxicitiy as well as toxicity integration into the LCA framework with harmonized impact indicators. Therefore, Backhaus et al. recently developed an artificial intelligence (AI)-based toolbox for in-silico assessment of the ecotoxicity of chemicals [403, 404]. 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 [405]. Furthermore, as we continue to expect to obtain fuel blends (such as KEAA) in FSC^2, 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 [406]. LCA has been applied to chemical conver-

sion systems on a molecular and process scale to guide catalyst design and electrochemical synthesis [299, 300]. 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 environnmental impacts. Therefore, in a combined process network flux analysis (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 [244]. 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) [301] and to evaluate whether and how DSM offers environmental benefit [302, 303]. 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 [304].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 [305, 306] and systematically reviewed product quality aspects for waste recycling within LCA [307].

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 [245]. 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 emissions efficiently. To assess the absolute environmental sustainability of fuels & chemicals, the LCA approach show be extended from the product-centric assessment of '1 MJ fuel', '1kg chemical' or '1 person-km mobility' 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 [308] , which is currently adapted for fuels and mobility systems.

Objectives

The methodology of Life-cycle assessment will be extended in order to better analyze the full range of sustainability impacts of fuels and to optimize fuels accordingly. In particular, the objectives are to:

- improve LCA-applicable methods for (eco-)toxicity assessment of chemicals, fuels and fuel blends by bridging data gaps via in-silico prediction tools
- 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

- develop new methods to optimize the transition from the current mobility and energy systems towards an absolute sustainable future within planetary boundaries
- extend the LCA methodology and planetary boundaries concept for socio-political implications for vital resources such as the water, energy and food nexus
- 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 direct liquid fuel cells (DLFCs) (see XY.). 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 Design will form the basis for the LCA assessment and LCA-based optimization. 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. 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, and apply it to the fuel & chemical supply chain transition. 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 deceeded. We will investigate the water-energy-food nexus from a social science perspective including political and cultural dimensions and questions of global justice.

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. 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 transistion 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 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).

4.5.5.4 Proposed Staff and Funding of SRA-RACS

Table 4.5.5.1: Proposed Staff in SRA-RACS

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Staff category			**Number of persons**				
Professors	0	0	0	0	0	0	0
Independent junior research group leaders	1	1	1	1	1	1	1
Postdoctoral researchers	2	2	2	2	2	2	2
Doctoral researchers	13	13	13	13	13	13	13
Other staff	0	0	0	0	0	0	0

Table 4.5.5.2: Funding Request for SRA-RACS

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff (Total for 4.5.5)	1143	1177	1213	1249	1286	1325	1365
Direct project costs (excluding staff)	150	150	150	150	150	150	150
Total instrumentation < €150,000	0	0	0	0	0	0	0
Total instrumentation > €150,000	0	0	0	0	0	0	0

4.6 Supplementary information on legal and ethical aspects of the research program

TMFB/FSC publications

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5 Structures and strategies in the Cluster of Excellence

5.1 Support of early-career researchers (Niklas von der Aßen | Abhishek Khetan)

The Integrated Fuel & Chemical Science Center (FSC^2) will continue investing in the development of early career researchers for facilitating the swift 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 for doctoral candidates, postdocs and "Advanced Talents". At RWTH, "Advanced Talents" denotes early-career PhD holders who are pursuing a tenured professorship. With a consistent and well-structured programme targeted at specific groups, CYA offers a diverse and contemporary range of personnel development services that support not only academic career paths but also professions in business and public services. Within CYA, the RWTH Doctoral (Postdoc) Academy offers doctoral (postdoctoral) researchers a wide range of transversal skills development courses as well as coaching and advising for systematic career planning, Each year, the two academies organize more than 300 free seminars, workshops and other events with over 3500 participants. These include training in scientific integrity, leadership, science communication, career orientation, societal translation, scientific writing and presentation skills. The current program of available courses is accessible online[AW5]. These complements the cluster's interdisciplinary program and imparts the necessary skills for collaboration.

Besides the CYA, the Center for Teaching and Learning Services (CLS) offers various modularized trainings, including the certificate program "Professional Teaching Competences for University Teaching" for researchers at all stages to expand their competences in teaching. To promote a common leadership and supervision culture, and to equip researchers with the necessary competences, the Center for Professional Leadership [AW2] (CPL) offers certificate courses ("Leading at RWTH"), mentoring and individual coaching for researchers and non-academic staff. 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 researches has resulted excellent outcomes at all levels. Some key examples are:

- The FSC established 17 new professorships at various levels (W1/W2/W3), including junior professorships with tenure-track. (Arning, von der Aßen, Backhaus, Boxx, Herres-Pawlis, Khetan, Lauterbach, Leicht-Scholten, Magnus, Mechler, Venghaus, Waldvogel, Wiegand, Zobel, Piccini, Leitner group,and Greiff). From these, Prof. von der Aßen has been promoted from a W1 to W3 position as the director of Chair of Technical Thermodynamics (LTT) at RWTH Aachen University (RWTH). Prof. Piccini has obtained a permanent position at Modena. Prof. Khetan has completed a successful interim evaluation and is being considered for a tenured W2 position.

- Several postdocs of FSC, who benefited from the extensive early-career support measures, have now won academic positions at esteemed institutions across the globe: Jun. Prof. Irina Delidovich (TU Wien), Jun. Prof. Tristan Becker (TU Dresden), Jun. Prof. Philipp Trotter (BU Wuppertal), Jun. Prof. John Linkhorst (TU Darmstadt), Assistant Prof. Artur Scheidtmann (TU Delft), Assistant Prof. Dominik Bongartz (KU Leuven), Prof. Changlong Wang (Beijing University of Technology). Dr. Andrea Hirsch won the NRW Rückkehrerstipendium 2024 to start her independent career at RWTH Aachen.
- FSC PhD Candidate Philipp Morsch is now group leader in the FZ Jülich. Nils Kurig won the Leopoldina fellowship.
- We established the FSC Research School under the guardianship of the FSC Steering Committee, which 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 such support measures, some of the Bachelors students were able to directly **”fast track”** to a PhD within the FSC.
- The FSC financially supported over a dozen international researchers who won the DAAD internships. We also financially supported several researchers (B.Sc/M.Sc./PhD/Postdoc) to visit other universities as well incoming researchers to work in the FSC.
- **first attempts of a research school: voluntary courses (not mandatory yet), a tailored program at CDS (statistics from Jenny Roseboom will follow) .... still to come**
- **Numbers on ”external” early-career researchers: all numbers from start of funding until 2023: 8 percent of PhD students from abraod, 28 percent of postdocs from abroad, all junior research group leaders from germany, 50 percent of junior professors from abroad, 3 percent of full professors from abroad**

5.1.2 Early Career Support at the FSC^2 Research School

To benefit from the continuity of the systematic framework provided by the FSC Research School established in the first phase, we will establish a similar associated FSC^2 Research School (FSC^{2}RS) operated by the FSC^2 Steering Committee. The FSC^{2}RS will facilitate the T-shaped growth of researchers at all levels: they 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 FSC^{2}RS's cluster specific activities, e.g., lecture series, weekly seminars, colloquia with external guests (FSC^2 Seminar), rotational lab courses, regular retreats, seasonal schools and young researcher conferences (see chapter 5.3). The FSC^{2}RS 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 FSC^{2}RS 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.

5.1.3 Measures of Early Career Development at the Different Stages

5.1.3.1 Undergraduate students (B.Sc./M.Sc.):

One of the FSC^2's most unique educational features are the numerous 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 bursaries for the Competence Area (CA)- and Translational Research Team (TRT)-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 FSC-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 FSC^2 will establish a new Masters course of study named Sustainable Chemistry and Technology, which will be aligned with its corresponding research domains. This is a measure to identify exceptional talents and expedite their development.

5.1.3.2 Doctoral researchers:

For doctoral candidates, the FSC^{2}RS 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 CAs and the TRTs, (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, international conference participation, and visiting periods at internationally renowned universities. It will also design an Individualized Qualification Curriculum for their candidate consisting of both mandatory obligations and recommendations. For example, all FSC^2 doctoral candidates a 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 consist of seminars and courses from the Doctoral Academy on, e.g., Scientific Writing, Time and Self-Management, Media Competence in Teaching and Presentation, Conference English, etc. We will encourage its doctoral candidates to also supervise smaller projects together with B.Sc. and M.Sc. students in order to develop leadership skills.

5.1.3.3 Postdoctoral researchers and tenure track professors:

Postdoctoral researchers will preferentially be recruited form outside to give fresh impulses and contribute additional competences. Along the with the support of a mentor within the FSC^2, 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. As described in XYZXYZ, FSC^2 will establish multiple new postdoc-level positions as JRG leaders. These leaders will be involved in teaching and have the privilege to supervise doctorates. They will co-supervise at least two Ph.D. projects together with a more senior PI. Upon recommendation by the FSC^2 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 [AW1], which are designed to attract outstanding graduates who have been abroad for at least two years. At least one third are awarded to female candidates. JPI fellows are provided with exceptional opportunities in terms of resources and networking to help them raise their research profile. Altogether, the structural measures both within and outside of FSC^2 will enhance the career prospects of postdocs for a successful promotion to a tenured professorship.

To further solidify our strength and promote young scientists, RWTH will establish two inter-institutional tenure-track professorships in co-ordination with Max Planck Institute for Chemical Energy Conversion (MPI CEC) and Forschungszentrum Jülich (FZJ). has established tenure track professorships in addition to junior professorships (limited to six years with the option of one additional year). The appointed tenure track professors have the opportunity to be appointed to a permanent position after successful evaluation. In addition, RWTH aims to offer all academic staff reliable and transparent employment prospects and to retain them when possible. This is reflected in the permanent employment concept of RWTH.

5.1.4 Early Career Coordination and Funding

A Steering Committee member (von der Aßen) is responsible for the management of the FSC^2 Research School and its support measures for early career researchers. This includes 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, CoE-specific staff development and individual career advising. He cooperates in close synchronization with the existing early career support structures at the RWTH Center for Young Academics. The early career support and its activities will be operationally supported out of the Cluster Office (0.5 FTE) with the following activities: coordination/monitoring of the mentoring of Ph.D. students, coordination of internships for undergraduates, and planning of the self-teaching and lab-rotation program for Ph.D. students. The personnel cost for the JRG “Toxicity Assessment and Prediction” is covered by FSC, whereas the JRG “Additive Fabrication of Novel Electrodes“ and JRG “Sustainable Life Cycles in Energy, Chemical and Process Engineering” as well as all new professorships in FSC[2] (see Section 5.2.1) will be funded by other sources (see Section 5.2.2). Moreover, all temporary professorships have the committed perspective to be tenured, either by commitment of the involved faculties and institutes or centrally by the RWTH rectorate. This commitment emphasizes the importance of the CoE to contribute to RWTH’s mission to operate as an Integrated Interdisciplinary University where natural sciences, life sciences and engineering sciences converge. Within the direct project costs, travel costs for seasonal schools, international lab visits, and registration fees for CDS and CPL are included. For each researcher within FSC, an annual budget of 2 k€ is foreseen. This budget is at the free disposal of the early career researcher from the Ph.D. student level on and can be spent for the various development tools (soft and science skills, summer school) within the framework to be established during the first year of the FSC. Since these costs are also covered by RWTH, please see Section 5.2.2 for detailed information. The requested instrumentation budget encompasses the start-up package for the (i) JRG “Additive Fabrication of Novel Electrodes” (for detailed description of this start-up package see Section 3.4.2.6) and (ii) the JRG “Toxicity Assessment and Prediction” (for detailed description of this start-up package see Section 3.4.3.6).

Funding:

JRG ”Electro-catalysts for Ammonia Fuel Cells”: 120k invest ”NH3 fuel cell test station” to be described in 4.5. + start-up Package ca. 65k + JRG Position

JRG ”High-through-put Catalyst Syntesis and Data Driven Testing”: start-up Package 75k

JRG ”AI in Kinetics”: 0 from DFG

JRG ”AI/ML Data Driven System Analysis and Modelling”: 0 from DFG

from Rother: “The establishment of a junior research group on biocatalysis at FZJ with a possible W1 appointment in the Department of Biology/Biotechnology at RWTH Aachen University will be considered. This junior researcher will be integrated into the research activities of FSC2.

Table 5.1.1: Funding Request for Early-career Support

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff	104	106	108	111	113	115	117
Direct project costs (excluding staff)	0	0	0	0	0	0	0
Instrumentation	255	0	0	0	0	0	0

5.2 Support of equity and diversity (Leicht-Scholten/Sebastian Bernhard)

Allgemeine Einleitung

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 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. In addition to developing concepts and measures to promote equal opportunities and diversity in research projects, RWTH's Gender & Diversity Consulting actively supports the consideration of gender and diversity aspects in research design and content. 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. Due to an increasing demand, the program lines have broadened significantly in the past years. Numerous former TANDEM participants now act as mentors for current participants. Allgemeine

Pläne/Ziele FSC

FSC is committed to implement and to further facilitate RWTH's vision and measures with respect to equity and diversity. In order to develop tailor-made measures for the cluster, the research group Gender and Diversity in engineering under the lead of Carmen Leicht-Scholten develops cluster-specific measures and monitor the implementation based on actual research in gender studies in STEM. Building on the university's gender equality initiatives FSC 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 to ensure transparent and quality-driven selection of new employees. Female researchers will be encouraged to take part in RWTH's TANDEM Mentoring Programs, complemented by the opportunity to get individual or dual career coaching to boost their careers. Moreover, dedicated financial support programs will be established such as the offering of re-entry positions for scientists returning from parental leave. To further ensure compatibility of family responsibilities and career, family support in collaboration with the Family Services Center, daycare facilities and short-term child-care services will be offered.

In the last CoE, FSC reached a share of XX % of female scientists among all disciplines and hierarchies. Through its many tenure track positions, FSC has achieved XX % female researchers on the junior-professor and professor level until 2023. At this stage, FSC comprises 40 % of female PIs in the core team, and two females out of six coordinators of the CAs in the steering committee. Nevertheless, FSC 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, FSC intends to recruit 30 % of its PhD students internationally by advertising the positions worldwide. While scientific quality will remain the primary recruitment criterion, FSC will prioritize ethnic diversity for tenure-track positions. To foster early intercultural awareness already at the PhD level, unconscious bias training will be mandatory for new PhD students.

To create a family-friendly research environment, FSC will provide its employees with a supportive digital infrastructure to ensure workplace flexibility. In addition to flexible and easy access to childcare opportunities and lab technician support for pregnant PhD candidates and Postdocs, particularly male PhD students will be encouraged to take parental leave.

Wissenschaftlicher Ansatz im FSC, Carmen Leicht-Scholten/Sebastian Bernhard

In addition to the aforementioned structural measures to support equity and diversity, this topic will be explored scientifically. Under the leadership of Leicht-Scholten, the CoE will advance research on this topic:

Gendersensitive science and technology studies acknowledge given interdependencies between scientific, technological, and societal development. In extensive literature research and analyses, the group of Leicht-Scholten identified and focused on two areas that allow the connection of Gender Studies to the research done in the cluster to establish a conceptual basis:

1. 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: Not only do women and

members of other marginalized groups share a greater burden of negative effects of, e.g., environmental degradation and climate change, but they further have less access to resources (including access to energy and mobility) and, additionally, are less involved in decision or development processes that could contribute to a form sustainable development that could take on related injustices. This emphasizes the need to adopt a holistic, gender-sensitive and intersectional perspective on sustainability in the research context of the cluster.

2. As the cluster is researching (fossil) fuels, the topic of petro-masculinity was identified as a further suitable subject to establish our conceptual basis. The term petro-masculinity highlights the fact that fossil fuels contribute to more than energy consumption and related profits. They further contribute to the formation of identities that construct masculinity and femininity oppositely and in a state of inequality, which perpetuates existing injustices. Furthermore, this form of identity formation is linked to political positions that reject measures to create gender equality on the one hand and measures to protect the environment on the other.

Taken together, the application of this second research area thus allows the transition to an identity-relevant level, which subsequently enables personal activation and thus creates an intrinsic motivation for sustainable transformation in addition to the extrinsic motivation in (1). In sum, this conceptual basis builds a transformative lens for the research conducted within the cluster 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 as well as motivates for ethical usage of research findings for societal benefit. Adopting this perspective enables the contribution to the sustainable development of fuels on the one hand, and on the other the establishment of a point of contact in thematic proximity to the employees of the cluster. Concerning the latter, the following preliminary work was also carried out to ensure that implementation was tailored to the project and in line with the reality of the employees: Following the system-theoretical approach to diversity management, the organizational diversity of the cluster was assessed focusing on the factors of gender, internationality, and position. While this offered first insights into the diversity and reality of the cluster, this perspective will be broadened for structural and scientific purposes. Accordingly, in collaboration with the Office for Data Protection at RWTH Aachen a novel study design was developed that aligns with the theoretical framework on diversity as conceptualized by Gardenswarts and Rowe's. This framework considers diversity along three dimensions: internal, external and organizational with personality at the center of diversity. The study, which is voluntarily and completely anonymous and non-traceable, allowed us to gain insights into the following dimensions of diversity: age, gender identity, cultural background, sexual orientation, migration background, care responsibilities, physical and mental health, visible and non-visible disabilities, family background, and international experience. Combined with the established theoretical background, this picture of the cluster's diversity can serve as the basis for an initial needs-oriented workshop that integrates these topics with the reality of the cluster and its employees. Anna Åberg from Chalmers University, a renowned international historian of technology with a gender-sensitive focus on energy and resource history, has already been recruited for a keynote and workshop on petro-masculinity and sustainable development. 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 the industry.

Based on these findings, the group of Carmen Leicht-Scholten has outlined the potential for further research on gender and diversity in the context of FSC². Specifically, the objective is to further explore and implement a systems-theoretical approach to diversity management within the FSC to (1) further contribute to the development of an inclusive research organization and culture, and thereby (2) contribute to the socially responsible and sustainable development of transformative fuels. In addition to extensive literature reviews, quantitative and qualitative studies, and hermeneutic efforts, practical actions that will result from the planned research have already been outlined. These include, for example, scientifically grounded workshops on ”Experiences of Discrimination in Scientific Research Organizations”, ”Inclusive Communication in Scientific Research Organizations” or ”Guidelines for Communication and Collaboration”. 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, promotes scientific excellence and innovation. Furthermore, it attracts diversity and excellence in human resource development, which, in turn, contributes to the fulfillment all the objectives of the CoE. Additionally, it enables effective knowledge transfer within the cluster research community, as well as to gender studies and even to industry.

5.2.0.1 Equity and Diversity Coordination and Funding

In contrast to the previous phase, the measures are accompanied by integrated gender and diversity research. Both are coordinated by Prof. Leicht-Scholten and carried out by a 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

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Funding category	**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
Instrumentation	0	0	0	0	0	0	0

5.3 Strategies for research data (Herres-Pawlis & Rother) and research software management and provisions for research infrastructures and instrumentation

As the amount of research data is strongly growing but at the same time extremely valuable, FSC^2 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 planss (DMPs), GitLab for code versioning, the RDM platform Coscine for handling and archiving FAIR (Findable, Accessible, Interoperable, Reusable) data [407], the electronic lab notebook eLabFTW, and the institutional repository RWTH Publications for publication of research data and software code. A university allowance of XXXXXXX was used to set up data steward positions in the Cluster of Excellences (CoEs) 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 FSC^2 are NFDI4Ing, NFDI4Cat and NFDI4Chem, in which RWTH respectivly FSC^2 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 have been 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 to discipline-specific curated repositories.

add text from engineers

NFDI4Cat has developed a controlled vocabulary [408] for digital catalysis where NFDI4Chem delivers Chemotion as ELN and repo as integrated, open-source solution for molecular data

[409]. For further chemical and catalytic data, RADAR4Chem has been established as multipurpose repository.

Contrary to the initial strategy of a single data steward responsible for the RDM measures of FSC, it has proved useful to establish a RDM supporting structure in the form of an interdisciplinary data steward team. The team supports researchers by defining RDM standards, explaining the FAIR principles [407], and supporting in the development of tailored DMPs. Currently, there are three data stewards who meet monthly with the managing director of the CoE. 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[407], the RDM policy applies to all FSC^2 researchers and addresses intellectual property, the use of data management plans, handling of metadata, data preservation, open access publications and deletion of data. Teaching and training efforts for FSC^2 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. With the implementation of DMPs valuable research data will be 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 the cluster and RWTH are already well equipped with RDM tools, the researchers 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 [11][3–4]. 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 ...) 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 37). 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 FSC^2 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.

5.3.0.1 Coordination and Funding of Research Data, Infrastructures, and Instrumentation Management

RDM measures are coordinated by the data steward team in close cooperation with the cluster office. RWTH will provide one FTE (E13-E14) of funding for the scientists involved in the Data

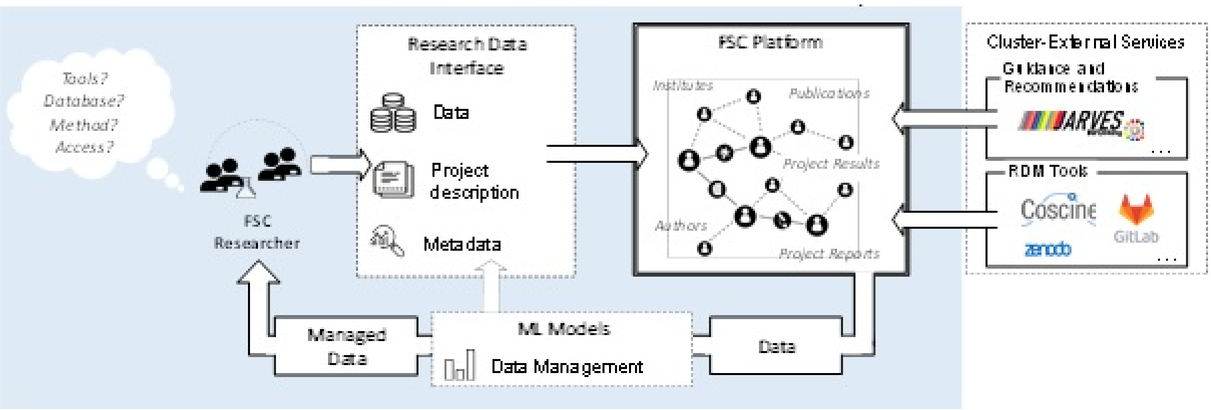

Figure 37: RDM concept within the cluster's platform.

Steward Team. In addition, 0.5 FTE (E13), also centrally funded by RWTH, is planned for the further development and maintenance of the internal communication platform. Direct cost include RDM software fees, IT-infrastructure (particularly server costs) as well as RDM trainings. All measures for the management of research data, infrastrucures and instrumentation will be financed centrally by RWTH, see Section 6.2.

Table 5.3.1: Funding Request for Research Data Management, Infrastructures, and Instrumentation

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Funding category		**Totals per year in thousand euros**					
Staff	0	0	0	0	0	0	0
Direct project costs (excluding staff)	0	0	0	0	0	0	0
Instrumentation	0	0	0	0	0	0	0

5.4 Management, governance (Lehrheuer), quality assurance(Isenhardt, Johanna Lauwigi)

RWTH's ambition is to be Germany's academic cornerstone for providing sustainable solutions that impact current and future challenges. The university has developed and uses its governance as an enabler of its vision and values and to serve its members, network partners and society. Guaranteeing responsiveness and the capacity for organizational renewal is key to the University's strategic development. This requires effective coordination, involvement, and commitment of all parts of the University and its partners.

RWTH's governance model makes use of an effective balance between collegial self-organization and top-down monitoring and directing. New ideas are initiated bottom-up through networks of PIs. Collegial self-organization in the institutes, faculties, centers and Profile Areas enables interdisciplinary research and convergence next to individual autonomy, creativity and freedom of disciplinary research. Various measures of the funding line University of Excellence, in particular the Exploratory Research Space and the Strategy Fund, facilitate and support these explorative processes and incubate them to a state where further implementation proceeds swiftly. The rectorate and faculties fulfill the formal hierarchical function of managing the processes of developing, organizing, and implementing a teaching portfolio and collaborative research. The final responsibility for developing the overall strategy of RWTH and allocating resources lies with the rectorate.

Decisions concerning appointments, structural development, and allocation of resources are the result of negotiations between the faculties and rectorate when those parties come together in the form of the Planning and Allocation Committee. Since Profile Areas and CoEs inform the Planning and Allocation Committee on a regular basis, suggestions, plans, and ideas based on their evolving roadmaps can be incorporated into the decision process.

The Planning and Allocation Committee is supported by the scientific Strategy Board. Using its scientific expertise, the Strategy Board evaluates upcoming topics, works out recommendations, and proposes resolutions to the Planning and Allocation Committee. The composition of the Strategy Board ensures that the University's interdisciplinary competence profile, strong ties with partner institutions, and the ambition to promote young academic talent are adequately represented. Permanent members are the speakers of the CoEs, representatives from the Profile Area, the FZJ, and other extramural research institutions located on Aachen premises. The group of young advanced talents, organized within the Center for Young Academics, delegates one permanent representative to the Strategy Board. Temporary members may be invited to join the Strategy Board when external expertise is required on specific topics. This broad participation ensures the sustainability and continuity of the board, as well as its ability to act flexibly.

A close exchange between the Planning and Allocation Committee and the Senate ensures broad acceptance and implementation of the RWTH strategy throughout the university. This is particularly important with regard to major developments and changes. Regular university-wide workshops also involve other key stakeholders in the strategic development. They are all empowered to act as ambassadors within the University.

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 FSC^2 network are based on the jointly agreed CoE's statutes, which describe all operational procedures.

The management structure of the CoE is illustrated in Figure 38. 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.

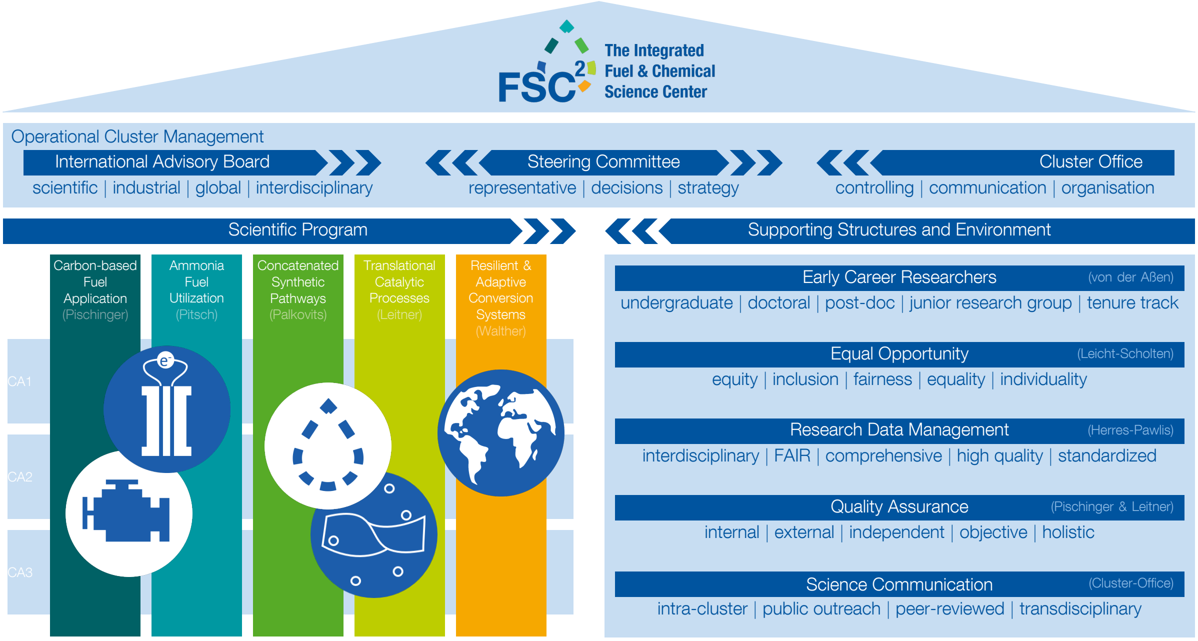

Figure 38: Management structure of the CoE

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 Pischinger 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 38). 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 spokepersons (Pischinger, Leitner) retirement will be within the next funding period, there replacements will be elected as foreseen in the clusters governance.

The 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 FSC^2, insuring a close alignment of the cluster's objectives and the demands of its key stakeholders. The rector of RWTH is member of the IAB to facilitate the progress of the cluster. The meeting of the IAB will take place during the annual International Conference held by FSC^2. Advisors who have confirmed their participation are listed below.

Table 5.4.1: International Advisory Board (IAB) of The Integrated Fuel & Chemical Science Center

Name	Company/University	Position/Department
	Industrial Advisors	
Dr. Jens Artz	Dechema	
Andreas Bulan	Covestro	R&D Manager
Dr. Marcus Bollig	VDA	Managing Director of the Research Association of Automotive Technology
Prof. Dr. Maximilian Fleischer	Siemens Energy Global GmbH & Co. KG	Chief Technological Expert
Prof. Dr. Thomas Garbe	VW	
Dr. Thomas Haas	Evonik	Director Marcomolecular Chemistry
Dr. Ralf Karch	Umicore	Head of Research & Development Precious Metals Chemistry
Evangelos Karvounis	Ford	Director Global Powertrain Research & Advanced Engineering
Dr. Michael Krüger	Bosch	Head of Development Diesel Systems
Dr. Lars Menger	BMW AG	Specialist for Fuels and Additives
Gesa Netzeband	DGMK	
Dr. Hermann Pengg	Audi AG	
D.Sc. (Tech) Teemu Sarjovaara	Neste Corporation	Head of R&D, Products and Applications Research and Development
Dr. Peter Sauermann	BP	Director BP Global Fuels Technology
Dr. Hans-Christian Schaefer	DBU	Leiter Referat Biotechnologie, Projektgruppe Energie
Dr. Nicole Schödel	The Linde Group	Head of Chemical Development and Services
Dr. Marie-Noelle Semeria	TOTAL S. A.	Senior Vice President, Group Chief Technology Officer
Dr. Karsten Wilbrand	Shell PLC	Senior Principal Scientist Mobility
	Scientific Advisors	
Prof. Claire Adjiman	Imperial College London	Faculty of Engineering, Department of Chemical Engineering

Continued on next page

Table 5.4.2: Caption

(Continued)

Name	Company/University	Position/Department
Prof. Paul Anastas	Yale University	Center of Green Chemistry an Engineering
Prof. Adisa Azapagic	The University of Manchester	Sustainable Industrial Systems
Prof. Alexis Bell	Energy Biosc. Institute	Chemical Engienering
Prof. André L. Boehman	University of Michigan	Department of Mechanical Engineering
Prof. Avelino Corma	Universidad de Valencia	Chemistry
Prof. Yiguang Ju	Princeton	Department of Mechanical Engineering, ERC
Prof. Jay Keasling	University of California	Chemical & Biomolecular Engineering
Prof. Katharina Kohse-Höinghaus	Uni Bielefeld	Department of Chemistry
Prof. Amit Kumar	University of Alberta	Department of Mechanical Engineering. Deputy Director, Future Energy Systems
Prof. Martyn Poliakoff	The University of Nottingham	Chemistry
Prof. Ortwin Renn	IASS	
Prof. Philippe Sautet	UCLA	Catalysis, Surface Chemistry, Materials
Prof. Greg Stephanopoulos	Massachusetts Institute of Technology	Biotechnology and Chemical Engineering
Prof. Bert Weckhuysen	Universität Utrecht	Chemistry
Prof. Tao Zhang	Dalian Institute of Chemical Physics	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 FSC^2. The CFO is the point of contact with the Deutsche Forschungsgemeinschaft (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.

5.4.2 Scientific Program Management and Fund Allocation

The backbone of the CoE are the Competence Areas (CAs) that were established in the previous phase of the cluster. In comparison to the previous CoE period, 5 SRAs will become a part of all CAs. The SRAs address the greatest scientific challenges. These will be handled by the different CAs using the knowledge already gained in Phase 1. This approach intensifies the interdisciplinary exchange within the cluster.

The TRTs were successfully established in the first funding period. Within the 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 funds, but no longer need to be embedded in the structure.

An annual internal peer review process was established during the previous CoE Tailor-Made Fuels from Biomass (TMFB) and successfully continued during the first funding period of the FSC. As part of the review process, the alignment of projects within the CAs and SRAs as well as corresponding funding allocations will be monitored and implemented.

Each PI's process will be evaluated by his or her peers through written review, presentation, and discussions with the scientific staff. Particular attention is paid to the progress of the projects. In addition, all project reports are evaluated by the Steering Committee. On this basis, the Steering Committee can take supportive measures, demand a reorientation of the projects, or terminate projects prematurely. The quality of the CoE can be ensured through a collegial, transparent, and cooperative culture. This allows the Cluster to adapt to a constantly changing scientific, economic, and social environment.

5.4.3 Supporting Structures and Environment

The Cluster Office is responsible for the coordination and implementation of the supporting structures. FSC doctoral students are supported during their doctoral studies by the measures described above, including the FSC Research School (von der Aßen , Section X) and Equal Opportunities (Leicht-Scholten, Section Y). The supporting structures for the FSC research environment are managed by the members of the Steering Committee. They include quality assurance (Pischinger and Leitner), science communication (Palkovits), and research data management (Herres-Pawlis).

Quality assurance

To ensure excellence in quality in a research project as interdisciplinary and diverse as this cluster comes with challenges. The previous cluster established an approach for quality assurance that goes beyond the obvious quantitative measure of research output by evaluating both the quality and quantity of publications. Based on this method, an environment was created for the researchers where the interdisciplinary work and cooperation within the cluster are especially valued[1].

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[1] Balanced Scorecard evaluation of The Fuel Science Center in 2022

Table 5.4.1: Caption

Description of one or two measures taken based on the outcome of the reports, the peer project evaluation, or the Balanced Scorecard. Based on the learnings from the former cluster, this cluster builds on a steady improvement using three monitoring tools that evaluate the quality of each project as well as the overall cluster research and cooperation:

- Quarterly scientific progress reports comprise research-related and financial reporting.
- Annual internal peer project evaluation assesses (i) scientific progress, (ii) cooperation within FSC, (iii) relevance for FSC, (iv) the scientific output, and (v) research data management.
- Combination of quantitative and qualitative evaluation methods performed by the institute Intelligence in Quality Systems at the Laboratory for Machine Tools and Production Engineering (Isenhardt) that inspect the inner perspective (e.g., with a balanced scorecard evaluation to quantify key indicators and 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.

5.4.3.1 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 FSC^2-developed pathways by Institut für Energie- und Umweltforschung Heidelberg gGmbH (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 Score Card) and the annual internal peer project review.
All measures for management of the CoE and quality assurance will be financed centrally by RWTH, see Section 6.2.

Table 5.4.2: Funding Request for Management, Governance, Quality Assurance

	2026	**2027**	**2028**	**2029**	**2030**	**2031**	**2032**
Funding category	**Totals per year in thousand euros**						
Staff	0	0	0	0	0	0	0
Direct project costs (excluding staff)	0	0	0	0	0	0	0
Instrumentation	0	0	0	0	0	0	0

5.5 Science communication(Isenhard), knowledge transfer and research-oriented teaching(?)

Intra-cluster communication (Isenhardt)

A central aspect of research is communication. Within large clusters like ours, it could be challenging for interdisciplinary teams due to their diverse backgrounds and expertise. Coordinating communication across the whole cluster often requires effective dissemination of information to enable collaboration and innovation. In the previous cluster, 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:

- Contact information for each researcher to facilitate easy connectivity
- Detailed information about every project within the cluster to encourage cross-disciplinary engagement
- A list of all cluster publications to enable cluster-wide research
- Dissemination of news
- Access to a fuel database to support ongoing research

As a central contact point within the cluster, this platform will be further optimized to users' needs. Additionally, the platform can be enriched with new features, for example to facilitate data management within the cluster.
Formally, intra-cluster communication will occur through coordination meetings on different levels (CAs, TRTs, general assembly, situational working groups). Intensification and documentation of intra-cluster communications will be supported by RWTH-hosted software communication tools such as Microsoft Office SharePoint. Swift and effective scientific cooperation across the different locations of FSC will be facilitated through a digital team communication tool (such as MS Teams, Zoom, Webex), in which teams organize themselves according to the CAs, TRTs, and situational communication teams.

Science Communication

RWTH Aachen believes that the central task of a university is not only to generate new knowledge, but also to transfer this knowledge to society. This includes initiating open dialogues in the wider community on the basis of mutual respect. For this purpose, new instruments (such as the Knowledge Hub) were developed as part of the Excellence Strategy. In today's increasingly complex world, with countless information channels and multimedia omnipresence, finding reliable information is critical. But it is becoming increasingly difficult to distinguish the true from the untrue, the relevant from the irrelevant. Universities like RWTH have a special responsibility in strengthening trust in sound research and its findings. We must share our expertise and transfer our knowledge to society in a way that is transparent and accessible. RWTH prides itself on being a modern university that actively participates in the social discourse by offering innovative and sustainable solutions, e.g. in the transformation of former coal mining regions. At the same time, we invite and listen to societal actors. This is the basis for a new form of responsibility and respectful scientific communication.

External Scientific Communication

As successfully implemented in the previous funding period, external scientific communication in the second phase of the Cluster of Excellence will also take place through the publication of scientific results in renowned international journals, book contributions, monographs and conference proceedings. Additionally, the FSC invite national and international scientists to participate in its own international conference in Aachen. The annual conference, which is organized by the FSC, has been known by two different names, ”Tailor-Made Fuels – From Production to Propulsion” until 2018 and ”Fuel Science: From Production to Propulsion” since then. The conference has consistently been a resounding success, with no instances of cancellation. Even during the global pandemic of 2020, the conference continued in an online format. A novel hybrid format was subsequently devised. This now permits other interested parties to attend the conference and participate in the presentations via a live stream. Its continued success has led to the decision to extend the conference into the next funding period.

Societal Communication

The society is constantly informed about the activities of the CoE on its website and the FSC Newsletter. In addition, an annual report is regularly published and available for everyone who is interested in the research activities of the FSC. The cluster represents itself also on exhibitions, like the ACHEMA and Hannover Messe. In the previous funding period, the cluster was also active on social media platforms, like Facebook and ResearchGate. The cluster’s social media presence has been augmented to encompass an Instagram profile, an X account, and a LinkedIn page. Energieagentur.NRW supports the dissemination of the research results of the CoE by for example organizing workshops.

Knowledge Transfer

At RWTH, transfer is based on the conviction that successful innovation requires research that leads to added value for the economy and society, and vice versa. RWTH understands transfer as the continuous exchange of ideas, knowledge, technologies, and people within RWTH, with partner organizations, societal groups and industry. Transfer is a central component of the RWTH strategy. The forward-looking, active approach to transfer includes the interaction of intellectual property valorization, industrial research cooperation, start-up support and the active involvement of highly qualified and creative people. It contributes significantly to building the profile of an innovative university that sees its role in helping to shape social change.

The greatest impact is achieved through collaboration with strategic partners, the expansion and integration of new, but also internationally visible fields of action in transfer:

- Scaling through collaboration with partners: Collaboration with strategic partners, such as the FZJ, MPI für Kohleforschung, MPI for Chemical Energy Conversion, and industrial companies increases the resources for successful transfer. For example, this can result in greater impact in the IP area, e. g. for the exploitation of life science technologies. Close integration with partners further strengthens RWTH's transfer position: bundling of IP portfolios and specifically integrating and connecting industrial partners.
- Quantitative increase: The number of inventions and spin-offs can be increased through active scouting of research ideas and results, which form the basis for later transfer. The communication of impact-relevant indicators enables the management of transfer activities, benchmarking and communication with society.
- New formats: RWTH transfer is characterized by novel concepts and transfer formats that drive and accelerate the continuous exchange between the transfer actors. A central contact point for companies at the university coordinates and further develops all aspects of long-term strategic cooperations. With the Collective Incubator, Frontier Workshops, Living Labs, Techathons, the Knowledge Hub, etc., high-impact transfer formats have been established.
- Translation, a new instrument complementing transfer at RWTH, is concerned with the practical development and adaptation of technology for specific applications. Through translation of excellent research, availability of unique infrastructure and the best talents, RWTH orchestrates the interaction of researchers, industry, start-ups and society to solve the grand societal challenges.

RWTH's success model is based on its ability to generate and transfer knowledge, thereby providing the foundation for future innovations.
This strategy is supported by the work of the FSC. With its scientific structure of CAs and research areas, the FSC offers an ideal basis for successful knowledge transfer. It has long been part of industrial alliances, such as the CAT Catalytic Center and the Ford Research Alliance, and part of multilateral application-related research networks, like BMBF: Kopernikus, Carbon2Chem®, BMWi: xME-Diesel, EU: Plastic Waste to Value; GreenSolRes, and ALIGN-CCUS. The cluster also provides assistance to its members in the establishment of new businesses. Prominent examples of this support include AixCape, S-PACT, hte, en2Aix GmbH, Ecotech GmbH, and eovent. The International Advisory Board is consulted to provide further advisory support to cluster members who wish to found a company.

Research-Oriented Teaching

RWTH's goal is to provide its students with an exceptional academic education, ensuring that they have an excellent grasp of the fundamentals of their discipline and are prepared for lifelong learning. The university 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. The use of case studies from society and business, as well as the application of solution-oriented learning methods facilitate autonomous action and critical reflection of practical experiences in science and business.

A Blended Learning environment was established in the first funding period of the CoE to educate early career researchers from various disciplines. In this manner, it is possible to ensure that effective integration into the FSC's extensive research portfolio 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.

5.5.0.1 Coordination and Funding for Science Communication, Knowledge Transfer, and Teaching

The activities in science communication, knowledge transfer, and teaching will be coordinated centrally by the Cluster Office. Based on the experiences of the current cluster, 1 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.

Table 5.5.1: Funding Request for Science Communication, Knowledge Transfer, and Teaching

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff	0	0	0	0	0	0	0
Direct project costs (excluding staff)	0	0	0	0	0	0	0
Instrumentation	0	0	0	0	0	0	0

6 Environment of the Cluster of Excellence

6.1 Strategic development planning at the applicant university/universities (Anika Linzenich, Brigitte Küppers

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 FSC 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 Clusters of Excellence (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. The CoE FSC brings together various disciplines, thereby facilitating research and the transfer of knowledge on contemporary fuel challenges. The integration of the cluster into the RWTH's profile areas was successfully achieved during the last phase. This is evidenced by the more than 200 publications that have been produced within the cluster. Thematic analysis of these publications reveals that they encompass a diverse range of topics, including those from the natural and engineering sciences, as well as those from the social sciences and economics, among others.

The CoEs are closely interlinked with RWTH's strategic objectives of the second funding line, University of Excellence (UoE):

- Objective 1: Leverage RWTH's interdisciplinary research culture
- Objective 2: Develop a value-chain of knowledge from teaching to transfer
- Objective 3: Nurture talents, empower people and boost teamwork
- Objective 4: Strengthen existing and building new alliances
- Objective 5: Tune the agile governance culture

With these five strategic objectives, RWTH aims 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 FSC is an integral component of RWTH's strategic objectives, fulfilling a pivotal role in training, promoting, and supporting young scientists in their careers. It also plays a crucial part in fostering an interdisciplinary research culture, forging new connections with industry and academia, and strengthening existing partnerships.

RWTH networks with external partners in various relevant research fields. It attracts internationally recognized scientists what intensifies its collaboration with external partners, such as Forschungszentrum Jülich GmbH, Fraunhofer-Society, DWI – Leibniz Institute for Interactive Materials, the University Hospital in Aachen, and Max Planck Society. The Jülich Aachen Research Alliance (JARA) was established for the purpose of facilitating inter-institutional collaboration with the FZJ, which resulted in a notable enhancement of interdisciplinary research initiatives. The so-called Campus Project was initiated for the purpose of fostering industrial partnerships, wherein scientists from industry and academia share research facilities. The MPI CEC and RWTH established the KOALA project in collaboration to translate scientific knowledge and expertise into practical applications. This interdisciplinary initiative facilitates the transfer of sustainable chemistry research and development to industry. Start-ups in their pre-founding phase can be supported by QuinCAT, an incubator which supports its members to bring their idea from technology readiness level (TLR) 4 to TLR 7. The formation of the FSC serves to reinforce the existing ties between RWTH, FZJ, and the MPI CEC.

The structural integration of the CoE into the participating institutions has facilitated the achievement of certain successes during the previous project phase. For instance, inter-institutional and interdisciplinary projects have been initiated as part of the cluster, like Power-to-MEDME-FuE, MIX-UP, Take-off, and Carbon2Chem©. Additionally, first start-ups were successfully founded (examples).

6.2 Resources provided by the institution(s)

6.2.1 Staffing

It is important to acknowledge the participating PIs, who have extensive expertise in the relevant research domains and methodologies, as institutional resources. It should be noted here that some of the principal investigators from the core team are affiliated with two institutions: RWTH and the Helmholtz Association (e.g., Palkovits), or RWTH and the Max Planck Society (e.g., Leitner). In the extra-university framework, the operational functions of PIs include the four directors of FZJ institutes and the three directors at MPI CECs. It is estimated that about 20 % of the researchers and technical/administrative staff at the participating institutes will be directly involved in the FSC scientific program. Personnel, which is engaged to FSC but not financed by the CoE, is listed in Table 6.2.1.

Table 6.2.1: Staff funded by the participating institutions

	Funded by host university	**Funded by participating institutions**	**Funded by other sources**
		Number of positions	
Professors and equivalent	32	5	2
Junior research group leaders and equivalent	5	?	0
Postdocs and equivalent	12	3	0
Doctoral researchers and equivalent	20	4	2
Total academic staff	69	12	4
Non-academic staff	37	13	0

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 6.2.2: New tenure track and lighthouse appointments generated within the FSC[2]

CA	Level Start /Tenure	Topic	Initial Funding	Sustaining Institution/Host	Model
1	W1/W2	Modelling & Simulation in Catalysis	RWTH	RWTH, Nat. Sciences	Succession
1	W2/W3	????	MPG Forschungsgruppe (CEC)	RWTH, Nat. Sciences	Tenure Track, interinstitutional
1	W3	Inorganic Chemistry and Electrochemistry	RWTH	RWTH, Nat. Sciences	Early Succession
2	W3	Sustainable Chemical Processes	RWTH	RWTH, Mech. Eng.	Early Succession
2	W3	Fluid Mechanics	RWTH	RWTH, Mech. Eng.	Succession
2	W3	Heat and Mass Transfer	RWTH	RWTH, Mech. Eng.	Succession
1	W3	New Methods for Organic Syntesis	RWTH	RWTH, Nat. Sciences	Succession
3	W3	Techn. Acceptance, Risk Communication	RWTH	RWTH, Arts & Humanities	Succession
2	W3	Energy Conversion	RWTH	RWTH, Mech. Eng.	Succession
1	W3	Molecular Science and Engineering	RWTH	RWTH, Nat. Sciences	Succession
1	W2	Catalyst Development	RWTH/ Helmhotz	RWTH/FZJ, Nat. Sciences	Tenure Track, interinstitutional
1	W3	Digital Chemistry	RWTH	RWTH, Nat. Sciences	Lighthouse Professorship
2	W3	Fuel Cell Beyond H_2: Electro Organic Molecular Conversion	RWTH	RWTH, Mech. Eng.	Lighthouse Professorship

6.2.2 Infrastructural Framework

The PI at the 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. For the FSC, the activities for its members are strategically coordinated via a virtual center to optimize the benefits of the collaboration. Additionally, the FSC has access to the infrastructure of its partner institutions, like the infrastructure at the FZJ, the infrastructure at the MPI CEC, and the facilities at the RWTH belonging to the profile areas ECPE, MTE, MatSE, and MSE.

The RWTH provides the FSC with FSC. The building has a laboratory space of 1000 m^2 and an office space of 600 m^2. The building has also enough space to host international guest researchers. For teaching and educational purposes, it also contains a lecture hall and several seminar rooms.

The Center for Mobile Propulsion (CMP) and the Center for Center for Next Generation Processes and Products (NGP^2) 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 NGP^2 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 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.

The MPI CEC provides the FSC with additional infrastructure. The MPI CEC has its own workshop, which provides the necessary support for the project in terms of the required processes. The laboratories and their high-quality equipment provide an excellent infrastructure for the FSC. The MPI CEC is a partner in NFDI4Cat and is dedicated to the collection of all scientific data. The collaboration with the two other departments (Prof. Serena DeBeer - Inorganic Spectroscopy and Prof. Siegfried Waldvogel – Electrosynthesis) and the scientific infrastructure at the MPI CEC, which encompasses electron microscopy, catalytic technologies, EPR, electrochemistry, and instrumental analytics in service groups, is possible at any time. Additionally, the MPI CEC serves as a coordinating institution for several BMBF-funded projects, including the Kopernikus project P2X, the hydrogen lead projects TransHyDE and H2Giga, and Carbon2Chem®.

6.2.3 Funding

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:

- “ACalNet”, the Aachen-California Network of Academic Exchange, was a DAAD-supported network between RWTH and three campuses of the University of California (Berkeley, Los Angeles, and Santa Barbara). The network’s main objective was the exchange of students and researchers in the fields of catalysis and NMR science. After this program expired, FSC maintained its tight relationships with the various UC locations and thereby mirror the recently US-financed graduate and faculty exchange program IRES “Training next generation U.S. researchers in advanced magnetic resonance at the chemistry industry interfaces”. Due to its great success, the application for a follow-up project is planned for this year.
- In the field of biorenewable-based energy engineering, the University of Alberta (UAlberta) has been granted the Future Energy Systems research initiative through Canada’s First Research Excellence Fund competition, a prestigious program of the Canadian government. RWTH and UAlberta are developing an institutional partnership, enhancing their collaboration through joint research projects, student and doctoral student exchanges, co-planned and delivered courses, and reciprocal research and teaching visits by professors.
- The Undergraduate Research Opportunities Program (UROP) will provide specialized research summer schools and internships at FSC research facilities. This well-established program predominantly attracts students from North America to Aachen.
- Through “CatchBio,” a government-funded research network in the Netherlands, TMFB has established a strong partnership that was continued between FSC and the “Netherlands Center for Multiscale Catalytic Energy Conversion.” The partnership will be also continued in the second phase of the FSC.
- The FSC has developed an annual exchange meeting comparable to the CatchBio cooperation with e-Refinery and VoltaChem. This partnership will be continued in FSC^2.
- The German Ministry for Education and Research has launched the “Kopernikus Projects for Energy Transition,” a series of major nationwide networks involving academic and industrial partners. One of these projects, Power-To-X, is coordinated by FSC PIs Leitner (RWTH) and Eichel (FZJ) in collaboration with DECHEMA. Complementing the FSC approach, this project focuses on the chemical storage and utilization of excess power through a combination of (co-)electrolysis and subsequent conversion of hydrogen, carbon monoxide, and synthesis gas using well-established catalytic processes. In another project, SynErgie, which aims at demand-side management in production and manufacturing processes, the chemical processes area is led by FSC PI Mitsos (RWTH).
- The “CAT Catalytic Center” is a long-term strategic collaboration between RWTH and the company Covestro. The CAT Catalytic Center has an over a decade old history currently approximately 28 young researchers and technicians. It is a successful example for translational research in public private partnerships. The research into catalytic CO_2 conversion has been of great significance in the development of a new industrial process for use in the polyurethane industry, which has subsequently been implemented on a large scale.

- RWTH is a collaborating institution within the European Doctoral Program on "Sustainable Industrial Chemistry – SINCHEM," which is hosted by the University of Bologna in Italy. SINCHEM's objective is two-fold: firstly, to facilitate collaboration between high-level academic and industrial teams across Europe and secondly, to encourage student mobility.
- refuel.ch, Renewable Fuels and Chemicals for Switzerland, is a project funded by the Swiss Federal Office of Energy's SWEET program. The project was fund-raised by the ETH Zürich. Its objectives are, among others, the development of an interdisciplinary understanding of robust and sustainable pathways for chemicals and fuels, and the delivery of a robust strategy to meet the Swiss demand on sustainable fuels. The 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 of the four institutions are currently members of the BioSC. The PIs from the FSC Blank, Herres-Pawlis, Jupke, Lauterbach, Mitsos, Rother, and Walther are among those involved.
- The Bio4MatPro competence centre combines the capabilities of the research and industrial landscape in Rheinische Revier and in NRW for the biological transformation of materials science and production technology. The common goal is the biological transformation of key industries such as textiles, chemicals, medical technology and consumer goods as well as in the field of lightweight construction. The FSC PIs von der Aßen, Blank, Jupke, Klankermayer, and Palkovits are involved in projects as part of this collaborative and practical research.
- Together with stakeholders from business, agriculture, research, education, local authorities and the public, the BioökonomieREVIER initiative is pursuing the goal of developing Rheinische Revier into a model region for sustainable economic activity with international appeal. As deputy of the executive board FSC PI Jupke is working with FSC PI Blank and Mitsos on the structural changes in the Rhenish mining region as a result of the phase-out of lignite and climate change.
- AUFBRUCH, which is financed by the BMBF, is a new graduate cluster that commenced this year. A total of 37 principal investigators (PIs) 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. PIs that are part of the FSC which are also partners of AUFBRUCH are Palkovits, Herres-Pawlis, Jupke, von der Aßen, Blank, Rother, and Walther.
- etos (Waldvogel)
- Hydriogeni, Norwegen (Pitsch)
- NEDO, Japan (Pitsch)
- KOALA is an interdisciplinary cooperation platform with the objective of translating scientific knowledge and expertise into practical applications. The initiative was established by the MPI CEC and the RWTH. Involved PIs from the FSC are Palkovits and Leitner.
- The SusChemSys doctoral network operates at the interdisciplinary intersection of chemistry and process engineering. Its doctoral students belong to various universities and external re-

search institutions in NRW. The academic partners include RWTH, the Max Planck Institute for Chemical Energy Conversion, the Max Planck Institute for Coal Research, Ruhr University Bochum, Bergische University Wuppertal, Dortmund University of Technology, Bielefeld University, Siegen University, the University of Cologne, and Westfälische Wilhelms University Münster. Six industrial partners are also involved in the network (ALTANA AG, Bayer AG, Evonik Industries AG, Henkel AG & Co. KGaA, Jowat SE, OQ Chemicals GmbH). The PhD students also work for PIs involved in the FSC, like Palkovits, Leitner, Klankermayer, and Herres-Pawlis.

- The future research renter catalaix: Catalysis for Circular Economy is a project that originated at the RWTH Aachen University in Germany and was selected as the winner of the Werner Siemens-Foundation's ideas competition, outperforming 122 other submissions. The award, valued at 100 million Swiss Francs, recognizes catalaix's potential to drive transformative change in the field of sustainable development. FSC PIs that are also involved in catalaix are Klankermayer, Palkovits, Blank, Mitsos, and Walther.

6.3.0.1 Coordination and Funding for Collaboration with External Partners

The activities in collaboration with external partners are coordinated centrally by the Cluster Office. The direct project cost including travel cost, e.g, for annual symposia with cooperation partners, are covered centrally by RWTH, see Section 6.2.

Table 6.3.1: Funding Request for Collaboration with external partners

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff	0	0	0	0	0	0	0
Direct project costs (excluding staff)	0	0	0	0	0	0	0
Instrumentation	0	0	0	0	0	0	0

7 Funding Request

Table 7.1: Total Funding Requested for the Research Program

Research Subunits	Funding category	Total* 2026-2032
Subunit A	Staff	
	Direct project costs (excluding staff)	
	Instrumentation	
Subunit B	Staff	
	Direct project costs (excluding staff)	
	Instrumentation	
Total		

[*] as detailed in tables 4.5.x.2; amounts in thousand euros

Table 7.2: Total Funding Requested for Structural Measures

Structural measures	Total* 2026-2032
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	

[*] as detailed in tables 5.1 to 6.3; amounts in thousand euros

Table 7.3: Total Staff Requested

	2026	2027	2028	2029	2030	2031	2032
Staff category	**Number of staff positions**						
Professors							
Independent junior research group leaders							
Postdoctoral researchers							

Continued on next page

(Continued)

	2026	2027	2028	2029	2030	2031	2032
Doctoral researchers							
Other staff							

Table 7.4: Total Funding Requested

	2026	2027	2028	2029	2030	2031	2032	Total
Funding category	**Totals in thousand euros**							
Staff								
Direct project costs (excl. staff)								
Instrumentation								
Total project funding								

Guidelines for Appendix:
Please include only the following information in the appendix to the proposal. Do not include or submit any other additional information/materials beyond those requested.
The appendix does not count towards the maximum 120 pages of the proposal. For the publication lists to be provided in sections 1 and 2, please note:

- Works which are not in the public domain are not considered publications and cannot be cited. An exception is made in the case of papers that have already been accepted for publication, in which case the manuscript and the editor's confirmation of acceptance must be enclosed as a separate PDF file and uploaded via elan (see instructions in the guidelines).
- Publications should be listed with their full title, and, where possible, with their persistent identifiers (e.g. DOI/Digital Object Identifier), preferably by stating the number, otherwise by naming the URL.
- Authorship must be cited in unaltered form in accordance with how it appears on the published works. Publications with multiple authors may be cited as follows: >first author, second author, et int, last author<.
- Please sort the reference lists in descending order by date of publication (i.e. the most recent publication first).
- Renewal proposals only: The works referenced in Categories A and B should mainly serve as a report on research performed within the first funding period of the Cluster of Excellence.

Details of quantitative metrics such as impact factors and h-indices will not be considered in the review. Please refrain from providing such data in the publication lists.
Guidelines for A.1:
Please provide a list of up to 25 scientific or scholarly papers published in peer-reviewed journals, peer reviewed contributions to conferences or anthology volumes, and book publications which, in your opinion, are the most important to have been produced by the principal investigators in the Cluster of Excellence. Open-access publications should be designated accordingly.

Estimation:

A Appendix

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

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

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:

A.3 The 25 most important additional qualification indicators

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.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

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:

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

Table A.5.5: Staff diversity – gender

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

A.5.2 Effects of the Coronavirus Pandemic