The Integrated Fuel & Chemical Science Center

Adaptive Conversion Systems for Sustainable Energy Carriers & Chemicals

Renewal Proposal EXC2186

Contents

Nomenclature

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Acronyms and abbreviations

5-HMF	5-hydroxymethylfurufural
AEM	anion exchange membrane
AESA	absolute environmental sustainability assessment
AI	artificial intelligence
AIA	Chair of Fluid Mechanics and Institute of Aerodynamics
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
CARS	Coherent Anti-Stokes Raman Spectroscopy
CCC-NEMD	Chemical-Color-Coded Non-equilibrium molecular dynamics
CEM	cation-exchange membrane
CEMC	cluster-expansion method calculations
CFO	Chief Financial Officer
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
D1PFC	direct 1-propanol fuel cell
D2PFC	direct 2-propanol fuel cell
DAC	direct air capture
DAFC	direct ammonia fuel cell
DBFC	direct borohydride fuel cell

DDEFC	direct dimethylether fuel cell
DDMFC	direct dimethoxymethane fuel cell
DEFC	direct ethanol fuel cell
DEGFC	direct ethylene glycol fuel cell
DFAFC	direct formic acid fuel cell
DFG	Deutsche Forschungsgemeinschaft
DFT	density functional theory
DGFC	direct glycerol fuel cell
DHzFC	direct hydrazine fuel cell
DLFC	direct liquid fuel cell
DMFC	direct methanol fuel cell
DNS	direct numerical simulation
DSM	demand-side management
DTFC	direct trioxane fuel cell
DUFC	direct urea fuel cell
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
EHS	environmental health & safety
EIS	electrochemical impedance spectroscopy
ESM	energetic span model
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 Spectroscop
FZJ	Forschungszentrum Jülich
GCE-DFT	grand canonical ensemble density functional theory
GCMS	gas chromatography and mass spectrometry
GDC	gadolinium-doped ceria
GHG	greenhouse gas
HAA	3-(3-hydroxyalkanoyloxy)alkanoic acid
HC	hydrocarbon
HPC	High Performance Computing
HR	high reactivity

HS	high-swirl
HT	high-tumble
HyFiT	hydroformylated Fischer-Tropsch
IAB	International Advisory Board
ICE	internal combustion engine
ICNP	iron carbide nanoparticle
IDT	ignition delay time
ifas	Institute for Fluid Power Drives and Systems
ifeu	Institut für Energie- und Umweltforschung Heidelberg gGmbH
IR	infrared
ISPR	*in situ* product removal
KEAA	ketone-esters-alcohol-alkanes
LAS	laser absorption spectroscopy
LBV	laminar burning velocity
LCA	life-cycle assessment
LES	large eddy simulation
LIF	laser-induced fluorescence
LR	low reactivity
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
NHC	N-heterocyclic carbene
NLP	natural language processing
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
rGO	reduced graphene oxide
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-AU	SRA “Ammonia Fuel Utilization”
SRA-CBFA	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
TOF	turnover frequency
TRT	Translational Research Team
UDE	universal differential equations
UV	ultraviolet
XCT	X-ray computed tomography
YSZ	yttrium-stabilized zirconia

Symbols

η_i	net indicated efficiency

Guidelines for chapter 1:

Section 1.2:

Please indicate the university that will administer the funds of the Cluster of Excellence. Where applicable, please list all other applicant universities.

Section 1.3:

Please indicate the Managing University's authorised spokesperson of the Cluster of Excellence. Up to two additional spokespersons may be listed here. In the case of spokespersons not affiliated with the Managing University, their respective institutions should also be named.

Section 1.4:

Please list all participating entities with which close cooperation is planned and which are to receive funds from the Cluster's budget (e.g. non-university research institutions, other universities, institutions in the public domain).

Section 1.5:

Please list in alphabetical order up to 25 researchers, including the spokesperson(s), who are significantly involved in the Cluster of Excellence and in the preparation of the proposal. Also indicate the principal investigator's respective location and institution, their field of expertise and their position (e.g. W3, W2 or W1 professorship, independent junior research group leader, core facility leader, etc.).

Renewal proposals only: Please highlight principal investigators who were not indicated as principal investigators in the establishment proposal by placing an asterisk (*) next to their names.

Section 1.6:

In these tables, please list those (external) institutional and individual cooperation partners who will engage in significant and sustained collaborations with the Cluster of Excellence. Institutional cooperations are usually based on a cooperation agreement; partner institutions contribute their own funds and resources to the cooperation, but they do not usually receive funding from the Cluster of Excellence.

Estimation: In total, 3 pages for this chapter.

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

1.3 Spokesperson(s)

Authorised Spokesperson of the Managing University
Prof. Dr.-Ing. (USA) Stefan Pischinger

Further spokesperson	Institutions
Prof. Dr. rer. nat. Walter Leitner	RWTH Aachen University Max Planck Institute for Chemical Energy Conversion

1.4 Participating Institutions

Participating institutions	Location
Forschungszentrum Jülich (FZJ)	Jülich
Max Planck Institute for Chemical Energy Conversion	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	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
15	Univ.-Prof. Alexander Mitsos, Ph.D.	Aachen, RWTH	Process Systems Engineering	W3/permanent

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(Continued)

No.	Principal Investigators	Location/ Institution	Field of Expertise	Position
		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 Aachen, RWTH	Synthetic Enzyme Cascades	W3/permanent
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.

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

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(Continued)

No.	Institutional cooperation partners	Location
3	Universidad de Valencia	Valencia, Spain
4	ifeu - Institut für Energie- und Umweltforschung	Heidelberg, Germany
5	King Abdullah University of Science and Technology	Saudi Arabia
6	NRW.Energy4Climate	Düsseldorf, Germany
7	ETH Zürich	Zürich Switzerland
8		
9		
10		
11		
12		

Guidelines for chapter 2:

Please provide a plain-language summary of the research and structural objectives of the proposed Cluster of Excellence, in both English and German (text only, max. 3,000 characters each, including spaces. Please do not use special characters or images).

Estimation: In total, 1 page for this chapter.

2 Summary of the proposal

2.1 English (max. 3000 characters incl. spaces)

Since the mid 20th century, crude oil and natural gas have “fueled” the Anthropocene – literally through production of liquid energy carriers for mobility and transportation as well as by providing the crucial feedstock of carbon and hydrogen for the chemical value chain. REF Despite world-wide efforts to reduce the associated greenhouse gas (GHG) emissions, the demand for crude oil is predicted to reach an all-time high in the coming years. The scenarios for the reduction towards net-zero GHG emissions comprise a range of measures centered around the global availability of renewable energy. The resulting defossilization of the energy system imposes challenges and opportunities for the sectors transportation and chemistry where direct electrification is difficult or even impossible and existing fleets and value chains have to be considered. REF Shaping a post-fossil era at the energy-chemistry interface requires novel research concepts and breakthroughs in fundamental science to develop disruptive technologies leading to major societal and economic transformations.

In this dynamic context crucial for a sustainable future, 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 on the molecular, device, and systems levels to understand, master, and design sustainable processes for harnessing renewable energy in chemical energy carriers and products.

The interdisciplinary Competence Areas, successfully established by The Fuel Science Center (FSC), and their effective interconnection form the backbone of the unique research framework of FSC^2 to adaptively address the challenges of the “defossilization” of energy carriers and chemicals. All research activities are allocated within Strategic Research Areas (SRAs) stimulating disciplinary progress. With the specific infrastructure of the partner institutions and the scientific profiles of the involved Principal Investigators, FSC^2 is ideally positioned to align groundbreaking science with focal technology options for post-fossil molecular energy carriers and chemicals. Continuing efforts focus on fuel design for low-carbon and low-emission liquid energy carriers. Ammonia is now included as molecular energy carrier and chemical building block. In addition to combustion, electrochemical devices for recuperating chemically stored energy are studied. 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 on a global scale.

2.2 German (max. 3000 characters incl. spaces)

Seit Mitte des 20. Jahrhunderts haben Erdöl und Erdgas das Anthropozän „angeheizt“ – im wahrsten Sinne des Wortes durch die Produktion von flüssigen Energieträgern für Mobilität und Transport sowie durch die Bereitstellung des entscheidenden Rohstoffs Kohlenstoff und Wasserstoff für die chemische Wertschöpfungskette. REF Trotz weltweiter Bemühungen, die damit verbundenen Treibhausgasemissionen zu reduzieren, wird die Nachfrage nach Erdöl in den kommenden Jahren voraussichtlich ein Allzeithoch erreichen. Die Szenarien für die Verringerung der Netto-Null-Emissionen umfassen eine Reihe von Maßnahmen, die sich auf die weltweite Verfügbarkeit erneuerbarer Energien konzentrieren. Die daraus resultierende Defossilisierung des Energiesystems bringt Herausforderungen und Chancen für die Sektoren Transport und Chemie mit sich, wo eine direkte Elektrifizierung schwierig oder sogar unmöglich ist und bestehende Flotten und Wertschöpfungsketten berücksichtigt werden müssen. REF Die Gestaltung eines postfossilen Zeitalters an der Schnittstelle zwischen Energie und Chemie erfordert neuartige Forschungskonzepte und Durchbrüche in der Grundlagenwissenschaft, um bahnbrechende Technologien zu entwickeln, die zu großen gesellschaftlichen und wirtschaftlichen Veränderungen führen. In diesem dynamischen Kontext, der für eine nachhaltige Zukunft entscheidend ist, generiert The Integrated Fuel & Chemical Science Center (FSC^2) Grundlagenwissen und neuartige wissenschaftliche Methoden für die Entwicklung anpassungsfähiger technischer Lösungen, um erneuerbare Elektrizität und Rohstoffe in einem Systemansatz in flüssige Energieträger und Chemikalien umzuwandeln. Die RWTH Aachen University und ihre strategischen Partner, das Forschungszentrum Jülich und das Max-Planck-Institut für Chemische En- ergiekonversion, integrieren ihre Kompetenzen auf der Molekular-, Geräte- und Systemebene, um nachhaltige Prozesse für die Nutzung erneuerbarer Energien in chemischen Energieträgern und Produkten zu verstehen, zu beherrschen und zu gestalten.

Die interdisziplinären Kompetenzbereiche, die von FSC erfolgreich etabliert wurden, und ihre effektive Vernetzung bilden das Rückgrat des einzigartigen Forschungsrahmens von FSC^2, um die Herausforderungen der „Defossilisierung“ von Energieträgern und Chemikalien adaptiv anzugehen. Alle Forschungsaktivitäten sind innerhalb von Strategic Research Areas (SRAs) angesiedelt, die den disziplinären Fortschritt fördern. Mit der spezifischen Infrastruktur der Partnerinstitutionen und den wissenschaftlichen Profilen der beteiligten Principal Investigators ist FSC^2 ideal positioniert, um bahnbrechende Wissenschaft mit zentralen Technologieoptionen für postfossile molekulare Energieträger und Chemikalien in Einklang zu bringen. Die fortlaufenden Bemühungen konzentrieren sich auf die Entwicklung von Brennstoffen für kohlenstoff- und emissionsarme flüssige Energieträger. Ammoniak wird nun als molekularer Energieträger und chemischer Baustein einbezogen. Neben der Verbrennung werden auch elektrochemische Geräte zur Rückgewinnung chemisch gespeicherter Energie untersucht. Die chemische Wertschöpfungskette wird explizit als ein wichtiger Anwendungsbereich für neuartige Synthesewege und katalytische Prozesse angesprochen. Die Analyse auf Systemebene wird als integrativer Teil entwickelt, um Designkriterien für Nachhaltigkeit und Widerstandsfähigkeit auf globaler Ebene bereitzustellen.

2.2 German (max. 3000 characters incl. spaces)

Guidelines for chapter 3:

Please provide a list of what you consider to be the most important research and structural objectives, up to a maximum of ten, which you intend to achieve through the Cluster of Excellence and by which its success should be measured.

Estimation: In total, a maximum of 5 pages for this chapter.

3 Objectives of the Cluster of Excellence

3.1 Background and Motivation

The reduction of GHG emissions, especially CO_2, continues to be one of the major global challenges. While renewable power generation is rapidly growing, mainly through installation of wind turbines and photovoltaic, their overall share in energy is still small (Lit). In fact, the highest share of renewable energy is still based on biomass (Lit). The dominating challenge for global usage of renewable electricity remains transport and storage. Here, synthetic liquid energy carriers ("fuels") can provide a key solution not only for the use in transportation and stationary heating systems but also for the usage in the chemical value chain. While water electrolysis as a first step from electricity to hydrogen as a chemical is established, the subsequent options for the conversion to platform chemicals and fuels are more divers, and remain a topic for research. Hereby, carbon sources range from biomass over direct air capture to point sources from industrial processes and waste. The combination with air-based nitrogen to obtain ammonia as an intermediate or final energy carrier and chemical is another option to be considered and recently applied in Saudi Arabia (Lit: NEOM). In order to address sustainability and resilience, the complete value chain has to be considered for fuels and chemicals on a global and holistic scale to overcome the limitations of today's technologies.

Because of its crucial role of liquid energy carriers in the transition to renewable energy and carbon sources in the mobility and transport sector, The Fuel Science Center has developed methodologies to define future fuels – the fuel design process – with the focus on the usage in internal combustion engines (ICEs). A unique research structure and approach was implemented, simultaneously optimizing novel production pathways and highly efficient combustion systems with low emissions, leading to so-called bio-hybrid fuel candidates. As a feedstock, renewable electricity was combined with bio- and CO_2-based carbon sources. Net indicated efficiencies of beyond 49 % have been demonstrated by molecularly controlled combustion systems using novel fuel candidate blends.

The uncertainty and diversity in the mobility and transport sector have rather increased than reduced, in particular on a global scale. REF Besides bringing new powertrain technologies like battery electric, hybrids, fuel cells, and hydrogen engines, the awareness of additional challenges has fostered: (i) existing vehicle fleets have to be considered in order to achieve the CO_2 targets (1.4 billion ICE-driven cars in 2030, Lit Bosch), (ii) the energy supply and transport have to be integrated on a global scale, (iii) the material supply with its circularity requirements has to be addressed and connected to the renewable energy flow, and (iv) resilience has gained importance as a boundary condition, including changes in the political situation. These aspects will further increase the complexity of the methodology and solutions significantly, triggering the necessity for adaption of the methodology.

When considering these emerging aspects, we propose to carry FSC with its unique interdisciplinary approach to a next level by (i) integrating the usage to chemicals into the Fuel Design

Process, (ii) addressing nitrogen and in particular ammonia as new substance into the Fuel & Chemical Design Process, (iii) extending the fuel conversion by considering fuel compatibility with existing vehicle fleets as well as energy conversion in fuel cells, and (iv) intensifying the usage of machine learning (ML). With FSC^2, RWTH Aachen University, the Max-Plank Society, and the Helmholtz-Association will bundle their interdisciplinary fields in natural science, engineering science, as well as social and economic science to provide the scientific basis for sustainable fuels and chemicals.

3.2 Vision and Mission

In context of this dynamic development of utmost importance for a sustainable future,

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.

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 to encompass their competencies on the molecular, device, and systems level to understand, master, and design sustainable processes to harness renewable energy in liquid energy carriers and chemicals.

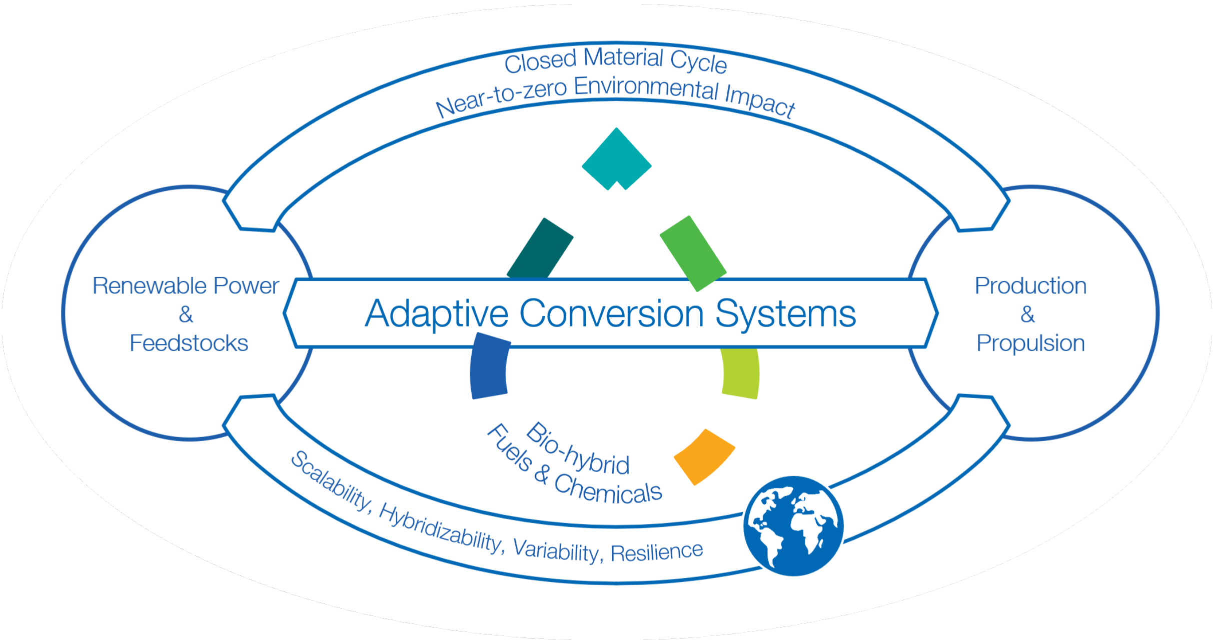

Figure 1: Vision of FSC^2

FSC^2 has its roots in the Cluster of Excellence (CoE) Tailor-Made Fuels from Biomass (TMFB) at RWTH. A unique interdisciplinary collaboration was established between combustion engineering, chemical engineering, chemistry, and biology using the intricate relation between combustion properties and the molecular structure of advanced bio-based fuels as common denominator. By the strategic development of projects and structural measures, a fundamental understanding of “fuel design” was successfully established for the first time. The subsequent CoE FSC was able to establish the broader field of “fuel science” internationally by overcoming disciplinary borders through composing the extended expertise of the network in interdisciplinary Competence Areas (CAs) according to the time- and length-scales of the molecular, device, and systems level. While carbon-based fuels were still at the center of the research activities, their application in advanced engine technologies and their “bio-hybrid” production based on biomass as well as CO_2 as alternative carbon sources could thus be envisaged. Expanding the research topics beyond the technosphere identified adaptivity as important design criteria to cope with the dynamics and variations in energy and feedstock supply at the interface between the energy and chemistry sectors.

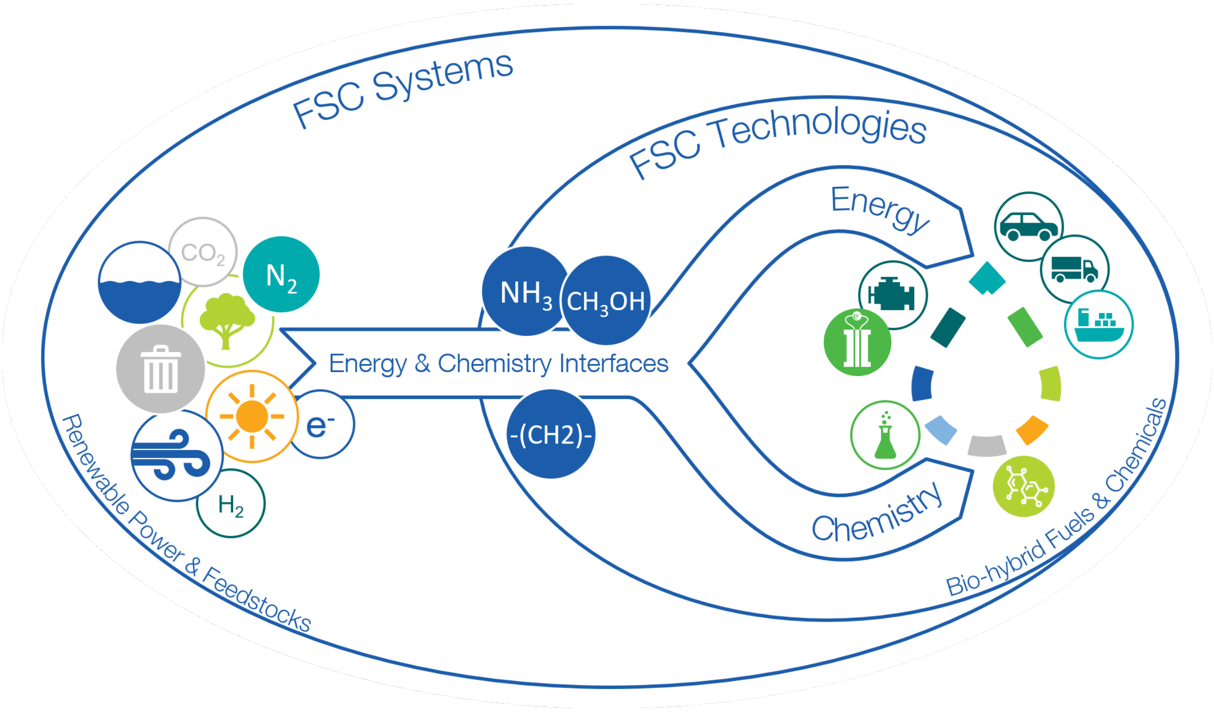

Figure 2: Mission of FSC^2

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 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 electro-chemical 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 Fuel & Chemical Design Process established by FSC.
- 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 efficiencies 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.
- How can chemical, biochemical, and electrochemical transformations for the manipulation of $C-O$ and $C-N$ bonds be interlinked to open concatenated synthetic pathways to fuels and chemicals? The transformations of bio-based C1 and N1 building blocks are usually addressed by the individual catalysis disciplines of molecular, heterogeneous, electro-, or biocatalysis. 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.

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 The Integrated Fuel & Chemical Science Center

Scientific Objectives
Exploration of chemo-, bio- and electro-catalytic pathways for the selective formation of C-H, C-C, C-O, and C-N bonds from renewable resources with the aim to integrate the individual transformations into optimized synthetic pathways for fuels and chemicals (concatenation) and their validation in view of feedstock variation and energy fluctuation in post-fossil value chains (translation).
Advancing the toolbox in experiment and theory for the investigation of complex catalytic reactions and processes to derive design principles from the molecular to the process level as input for and in response to the interdisciplinary analysis in the Fuel & Chemical Design Forum.
Mitigate carbon emissions from existing vehicle fleet by developing bio-hybrid fuel based molecularly-controlled engine concepts that can be retrofitted to existing combustion systems enabled through advanced technologies for combustion and aftertreatment systems with energy conversion efficiencies beyond 50 % and near-zero pollutant emissions.
Develop carbon- and ammonia-based fuel cell concepts and ammonia-fueled combustion engines for new passenger vehicles, heady-duty, and marine applications enabled by fundamental understanding of the involved thermochemical and electrochemical processes
The fuel and chemical design optimizes the overall conversion performance, accounting for fleet-compatible and novel propulsion concepts and co-production of chemicals and fuels; this is done by developing and employing cutting-edge methods from propulsion equipment design, production process development, and machine learning.
System integration of the developed fuels, processes and pathways is enabled by interdisciplinary assessment and optimization of resilient and adaptive intersectoral conversion systems based on systemic risks, stakeholder perspectives, policies and sustainability criteria.
Structural Objectives
The “Fuel Science Center” 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 the FSC through 8 reappointments of established lighthouse professorships, and 5 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 the FSC Research School.
A coherent mentoring program and recruitment policy ensures at least 30 % female researchers across all disciplines and hierarchies of FSC.

Guidelines for section 4.1:

Please describe the research objectives of the Cluster of Excellence. Outline the fundamental approaches, methodologies and measures with which you will pursue your objectives. What particular challenges will the Cluster of Excellence address? In what areas will the research conducted in the Cluster of Excellence bring about key advances in terms of the current state of knowledge? What added value is expected through (inter-)disciplinary collaboration? In what ways will the Cluster of Excellence have an impact on the long-term development of the research area and/or the establishment of new research areas? What makes this Cluster of Excellence unique internationally? How is the proposed Cluster of Excellence positioned in terms of its research profile in relation to existing groups and institutions, both in Germany and in other countries?

Estimation: In total, a maximum of 2 pages for this section.

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.

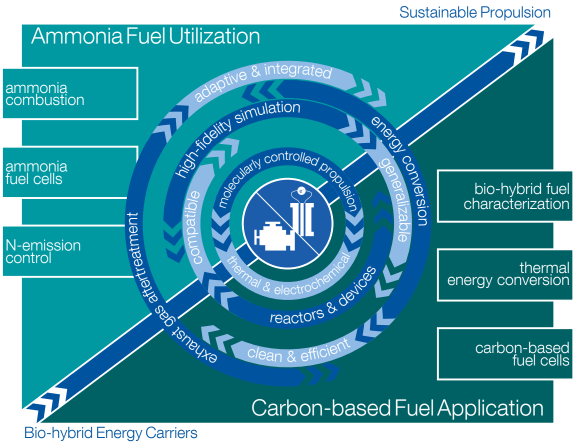

***Figure 3:** Joint methodologies and targets of SRA "Carbon-based Fuel Application" (SRA-CBFA) and SRA "Ammonia Fuel Utilization" (SRA-AU)*

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-CBFA), the fuel design process successfully established in the previous phase of 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-AU), 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 molecular fuel cells will be envisaged focusing on thermodynamic efficiency, emission analysis and control, engine components, and systems integration.

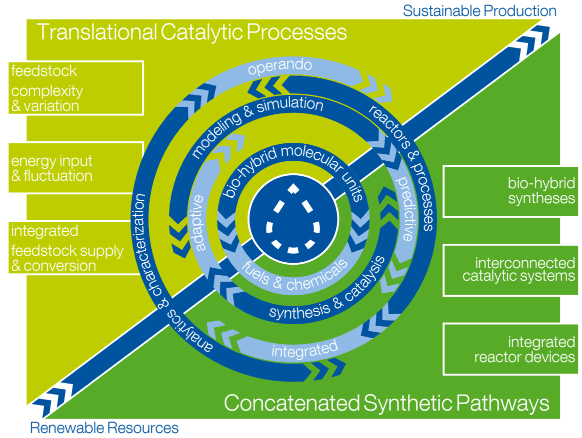

Figure 4: Joint methodologies and targets of SRA "Concatenated Synthetic Pathways" (SRA-CSP) and SRA "Translational Catalytic Processes" (SRA-TCP)

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-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-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 energy conversion, the two SRAs in production share certain common experimental techniques and modeling and simulation methods creating a synergistic toolbox.

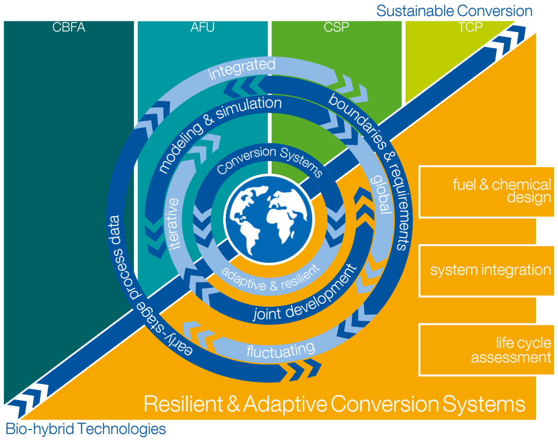

Figure 5: methodologies and targets of SRA "Resilient & Adaptive Conversion Systems" (SRA-RACS)

In 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.

Task forces will be formed for common topics and techniques with the potential to cross-fertilize the progress of the SRAs. This includes for example methods for the preparation and characterization of materials and interfaces including the analysis of dynamic processes under operating conditions, the integration of production pathways and propulsion properties for the C-based fuel design, or 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

- RWTH, MPI, FZJ => unique/strong
- Large scale projects: here FUNDAMENTAL, sonst eher translational
- Internationally leading: similar programs only on individual parts (name important ones), not holistic; partnerships
- Evidence: conference chairs, journal Editorial Boards?

aus FSC Antrag: The challenges and opportunities associated with a transition of the energy system and the use of non-fossil raw materials has led to major research initiatives world-wide. Rooted in its unique profile, in the scientific progress, and in the collaborative structures developed within the Cluster of Excellence “Tailor-Made Fuels from Biomass (TMFB)”, RWTH and its partners are ideally positioned to establish the “Fuel Science Center” as a national lighthouse and an internationally leading scientific environment in this highly competitive field. Targeting “fuels” as central pivot to interconnect the energy, mobility, and chemistry sectors allows the definition of common goals and a coherent research strategy for scientists at all career levels with diverse, yet complementary and synergistic expertise. The strategic partnership between RWTH, FZJ, MPI KoFo, and MPI CEC provides an excellent infrastructure and a critical mass of leading scientists, capitalizing on the individual profiles of the institutions within the German scientific landscape. While a number of research institutions world-wide focus on either the conversion of renewable energy into chemical storage materials or the development of alternative propulsion systems, the integration of both fuel production and propulsion systems in one common research framework is quite rare. Apart from the CoE TMFB, one of the very few large-scale initiatives embracing production and propulsion is the recently launched Co-Optima Initiative started by the US Department of Energy (DOE) in March 2016 [CO]. The initiative intends to “combine the previously independent areas of biofuels and combustion R&D, bringing together two DOE Office of Energy Efficiency & Renewable Energy research offices, nine national laboratories, and numerous industry and academic partners to more rapidly identify commercially viable solutions" [COa]. Current publications from this program deal mainly with the assessment of biomass-derived blending components for compatibility with existing engine concepts, infrastructures, and production routes [Du17]. The Co-Optima consortium has already indicated a strong interest to enter into collaboration with FSC in case of its approval. The potential for a pivotal international position of FSC in this research area is demonstrated inter alia by its strategic links to major research institutions and scientific partners through its Scientific Advisory Board (see Section 4.3). This includes the Joint BioEnergy Institute (JBEI; San Francisco, USA) [BE], the Sustainable Energies Program at the Dalian Institute of Chemical Physics (Chinese Academy of Sciences, Dalian, China) [DICP], the Netherlands Center for Multiscale Catalytic Energy Conversion [MCEC], the Engine Research Center at the University of Wisconsin (Madison, USA) [ERC], the Center for Sustainable Chemistry at University of Nottingham (UK) [CSC], and the Center for Process Systems Engineering at Imperial College (London, UK) [PSE]. Based on the fundamental insight and methodological progress, FSC is able to act as a motor for translational research activities transferring knowledge into innovation. In addition to focused industrial projects aiming at implementation, this is exemplified in particular by coordinating roles in large scale national academic-industrial networks such as the Kopernikus project "Power-to-X" and the BMBF initiative "Carbon2Chem®". It is also reflected by the strong commitment of representatives from companies covering the entire value chain from energy systems to car manufacturers in the International Advisory Board (see Section 4.3.1).

Guidelines for section 4.2:

Please indicate the main preliminary work, carried out by currently or previously funded local or regional research groups, for example, on which the Cluster of Excellence is based.

Renewal proposals only: Please include a concise description of the Cluster's most relevant achievements during the first funding period, also with regard to the objectives defined in the establishment proposal.

Estimation: In total, a maximum of 1.5 pages for this section.

Content: Only a short version is required here. Detailed descriptions shall be implemented in section 4.5.

4.2 Preliminary and previous work

In the previous phase, FSC has established a unique and world-leading research platform defining the concept of “fuel science” for the production and use of carbon-based liquid energy carriers in propulsion systems based on ICEs. This has been achieved on the one hand by the scientific progress of the individual Principal Investigators (PIs) in their respective disciplines and on the other hand by creating a culture of interdisciplinary collaboration. Disciplinary competences could thus be synergistically integrated ranging from fundamental knowledge on the molecular level, through the design and demonstration of advanced devices, to multifactorial systems analysis of sustainability criteria.

A central element for the collaborative efforts was the FDP aiming at the identification of promising target structures for sustainable fuels integrating their production route with the performance in the propulsion system REF (ANGEW REVIEW; scientific objectives #5). Recognizing that maximizing carbon efficiency and minimizing energy supply are essential design criteria for the production processes, “bio-hybride” molecules were defined to explore the synergistic potential of biomass and CO_2 as carbon feedstocks. Integrating innovative synthetic methods for catalytic CO_2 conversion with biomass-derived building blocks opened unprecedented synthetic pathways to fuel targets beyond established products (scientific objective #1). The potential for simultaneous gain in efficiency and reduction of emission levels was demonstrated for such new fuels when combined with advanced engine concepts and technologies (scientific objective #4).

Examples to highlight the interdisciplinary approach include the production of cyclic acetals combining catalytic CO_2 hydrogenation with bio-based alcohols as substrates by judicious combination of bio-catalytic and chemo-catalytic transformations [REFs Klankermayer/Blank/Rother & Jupke]. The adaptive synthetic pathway allowed for systematic structural variation of the bio-based component enabling detailed studies of structure-performance relationships in established and advanced engine technologies providing unprecedented insights in combustion mechanisms [REF Klankermayer/Pischinger/Pitsch]. In particular, engine concepts exploiting a combined use of low and high reactivity fuels (“molecular torch (MT) and molecular spark (MS)”) were shown to reach ultra-high thermal efficiency of up to 50 % [REF]. Another example is the production and use of long-chain alkane/alcohol mixtures where FSC research comprised all aspects from catalytic production, over combustion properties and materials compatibility, to a systems analysis of environmental parameters [REF Nature Energy].

The detailed insight derived from such iterative studies was combined with advancements in modeling and simulation techniques as basis for mathematical optimization methods across all levels (scientific objectives #2 and #6). This was successfully demonstrated for the holistic design of a bio-hybrid fuel blend comprising the newly developed process network flux analysis (PNFA) as the best compromise between CO_2 reduction, costs, and other life-cycle assessment (LCA) indicators such as land use [REF]. Challenges and opportunities arising from the use of electricity from renewable sources as the primary energy input for the production processes were addressed inter alia by strategically integrating the field of electrocatalysis on a molecular and device level (scientific objective #3). [EXAMPLES PALKOVITS, MAYRHOFER, WESSLING] These examples are provided pars pro toto to illustrate the collaborative spirit of FSC based on the disciplinary excellence of the PIs outlined in detail in the sections "previous work" in Chapter 4.5. The adaptive structure of FSC has been successfully used to integrated associate PIs at various career stages and to ensure a healthy mix of continuation and rejuvenation of a divers team of researchers team on all levels (structural objective #3 and #4). The seamless integration of strategically planned appointments at different faculties and institutions demonstrates the pronounced structural impact of the cluster (structural objective #2). The obvious benefits for scientific progress have provided an intrinsic driving force for new forms of structural collaborations between RWTH Aachen University, the Forschungszentrum Jülich, and the Max Planck Institute for Chemical Energy Conversion (structural objective #1). The resulting tight network has been instrumental in establishing a number of important large-scale collaborative projects with strong translational components (ReDiFuel, CatalAix, Helmholtz-Cluster Wasserstoff HCH2) or even directed to implementation (Kopernikus Power-to-X, Carbon2Chem, NaMoSyn).

The objective-oriented successful demonstration of individual scientific excellence, interdisciplinary team spirit, and institutional collaboration in FSC provides a strong basis for the generation of fundamental knowledge and methodological know-how in FSC^2 to enter new directions in terms of energy conversion technologies and molecular diversity of bio-hybrid products within the dynamics of a rapidly changing global system.

Scientific Objectives Erstantrag:

- Adaptive synthetic pathways are enabled by homogeneous, heterogeneous, bio- and electrocatalysis to integrate renewable energy with alternative carbon sources for a broad molecular diversity of bio-hybrid fuel targets, which are iteratively identified and developed via structure-performance correlations together with combustion science.
- Synergistic progress in experimental methods and modelling and simulation techniques provides unprecedented insights into molecular interactions that determine on the one hand the intrinsic pathways of combustion processes and on the other hand the structure and dynamics of catalytically active sites.
- Challenged by the fluctuating supply of renewable energy and carbon feedstocks, scalable and modular reactor concepts allow for bio-hybrid fuel production processes with high yield and selectivity over a wide range of boundary conditions.
- Molecularly controlled engine concepts are enabled through advanced technologies for combustion and aftertreatment systems and achieve bio-hybrid fuel-based propulsion with energy conversion efficiencies beyond 50 % and near-zero pollutant emission.
- The fuel design process identifies molecular fuel structures and co-products jointly with the required intensified chemical conversion processes and novel engine technologies to optimize overall conversion and propulsion performance.
- Interdisciplinary system-level analysis provides an integrated framework to assess and optimize the dynamic cross-sectorial integration of the electricity and fuel sectors based on multicriteria evaluation of economics, environmental impacts and stakeholders' perceptions.

The most promising bio-hybrid fuel candidates identified in FSC's iterative FDP can be divided into three groups. Firstly, fuels that primarily have advantages in terms of the synthesis process, where as much CO_2 as possible is coupled back into the new molecules (link bio-hybrid synthesis). The molecule groups dioxolanes and dioxane as well as methyketones should be mentioned here in particular [source Klankermayer & Blank]. The second group is primarily derived from the combustion properties. Here, for example, fuels with a high octane number and high burning velocity for spark-ignited combustion systems as well as fuels with a high cetane number and a certain proportion of oxygen-containing molecules for compression-ignition combustion have emerged as advantageous.zu trivial? more Details on Molecularly Torch & Spark, high & low reactivity fuels

The third group consists of fuel blends that were identified from the system analysis PNFA as the best compromise between CO_2 reduction, costs, and other LCA indicators such as land use.

To 50% target: The continuous co-optimization of the engine and the fuel yielded an increase of the engine efficiency and near-to-zero engine-out emissions over the years. In particular, the selection of suitable single fuels and fuel combinations enabled both an increase of the compression ratio (CR) and a decrease of the emissions to increase the efficiency. We did significant steps to achieve our target for an energy conversion efficiency of 50 %, and we are convinced that our next scheduled development steps will achieve our target until the end of the FSC funding period.

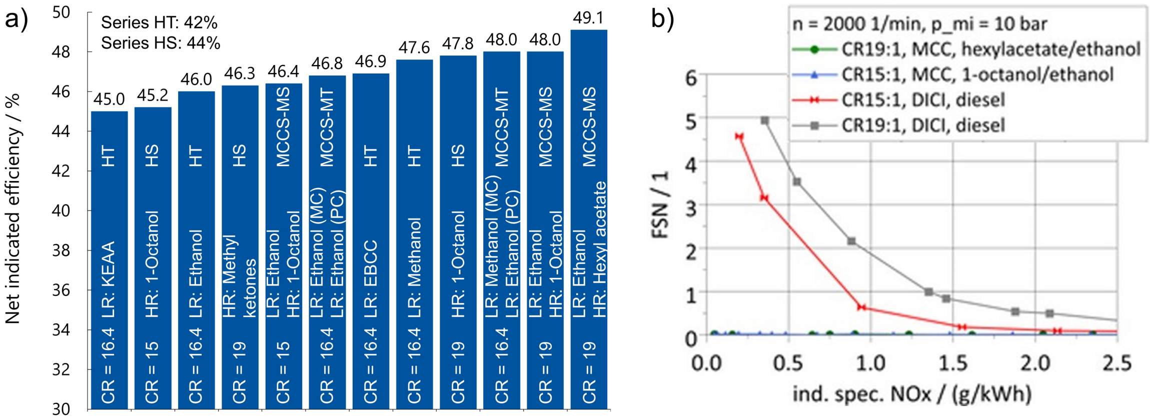

Figure 6: a) efficiency walk and b) NO_X-soot trade-off using various compression ratios (CRs), high reactivity (HR) and low reactivity (LR) fuels, high-tumble (HT) and high-swirl (HS) engines, molecularly controlled combustion systems (MCCSs), molecular torch (MT), and molecular spark (MS).

Guidelines for section 4.3:

Outline the chosen structure of the research programme, for example with reference to overarching topics or research areas and the essential links between them. To allow for the varying needs of different subject areas, there are no specific guidelines as to the structure of the research programme: it may be split into subunits or structured in another way, and the subunits denominated as needed (e.g. “areas”, “streams”, “classes” etc.). If applicable, a detailed description of the individual subunits should be provided in section 4.5.

Estimation: In total, a maximum of 1.5 pages for this section.

Content: Point out CAs as success.

4.3 Structure of the research program

The successfully established concept of interdisciplinary CAs and their effective and dynamic interconnection now form the backbone of the unique research framework of FSC^2 to address adaptively the challenges resulting from the "defossilization" of energy carriers and chemicals. The central achievement of the 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.

Now, all research activities and projects are allocated within SRAs where they absorb and vice versa stimulate the disciplinary progress of the individual PIs, thus constantly augmenting the CAs (Figure 7). 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, the fundamental mechanisms of electrochemical ammonia activation for energy or synthetic applications, as well as the seemingly contradicting goals of integration for process chains and flexibility of individual process steps.

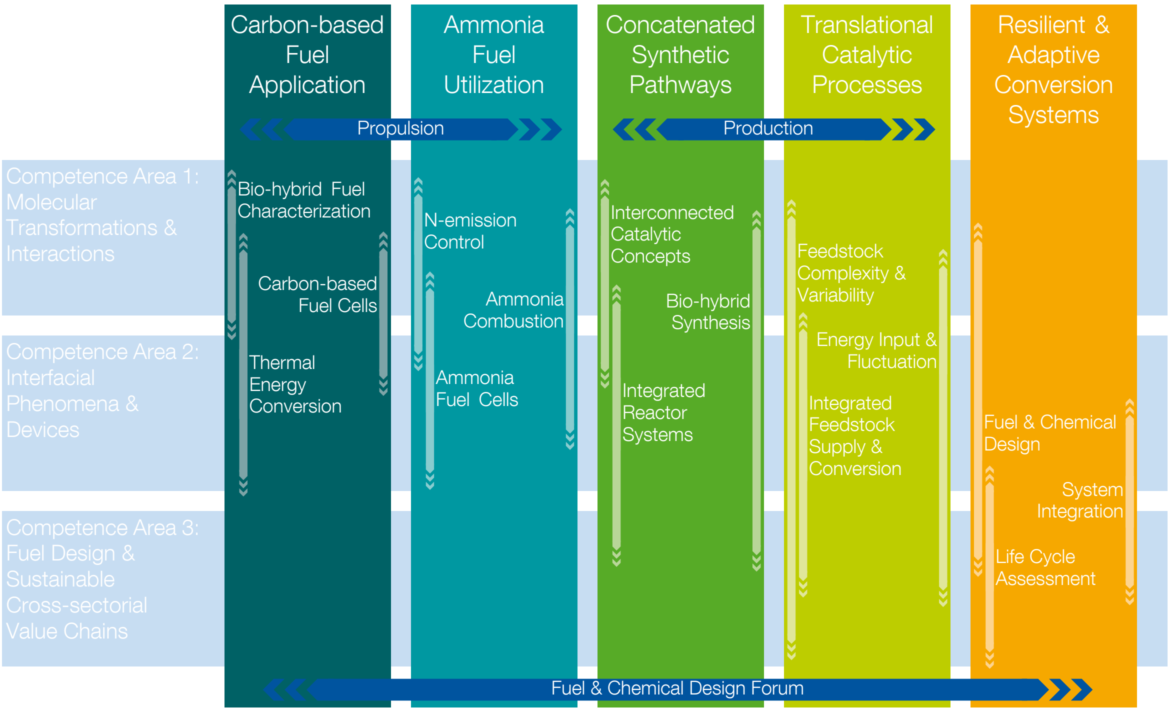

Figure 7: The integrated framework of the five Strategic Research Areas (SRAs) embedded within the Competence Areas (CAs).

Guidelines for section 4.4:

Outline the research profiles of the principal investigators. How will the principal investigators, staff and the cooperating partners contribute to achieving the Cluster's research objectives? Explain which other individuals and institutions are currently involved or will be involved in the future according to your current plans. When choosing principal investigators, staff, and cooperation partners, appropriate consideration should be given to diversity.

Renewal proposals only: Please include a concise synopsis of these aspects relating to the first funding period.

Estimation: In total, a maximum of 3 pages for this section.

4.4 Staff and institutional composition of the Cluster of Excellence

The 25 core Principal Investigators (PIs) represent the three Competence Areas (CAs) and define the thematic focus within the Strategic Research Areas (SRAs). The project work is, however, 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 4 researchers from RWTH and one from MPI CEC newly to the FSC PIs (💧) 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. 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 synergy across the institutions. A particular strength of the consortium in this context results from the fact that a number of 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, a Humboldt professorship as well as a Heisenberg Professorship, 5 ERC grants (3 advanced, 2 starting), and a number of 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).The PIs cover all academic career stages as basis for the longterm development of the research area.

In FSC^2, 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 and the environment will be enriched with complementary knowledge and methods. The FSC^2 foresees the integration of further associated researchers depending on the temporary formation of translational projects with flexible fund allocation. This adaptive process results in a CoE structure with a stable core allowing at the same time for flexibility where required.

In SRA-CBFA and SRA-AU, 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'

Table 4.4.1: Cooperation matrix

■ main activity
□ supporting activity
◉ SRA coordination

Researcher's Institution & Main Competence		Carbon-based Fuel Application			Ammonia Fuel Utilization			Concatenated Synthetic Pathways			Translational Catalytic Processes			Resilient & Adaptive Conversion Systems		
	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 Systems	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 | ◇ new FSC member | 💧 strategic FSC appointment competence in fuel injection, spray and mixture formation, in-cylinder fluid dynamic and combustion process (Kneer, Schröder, Pitsch, Pischinger), with Prof. Boxx● for the methodological competence in laser spectroscopy and Prof. Schmitz adding expertise in tribology and hydrodynamics. 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), with Prof. Leonhard adding competence in quantum chemistry and molecular dynamics. 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 PIs targeting the production processes in SRA-CSP and SRA-TCP cover competences in heterogeneous catalysis (Palkovits), homogeneous catalysis (Bolm, Klankermayer, Leitner, Schoenebeck), and biocatalysis (Blank, Herres-Pawlis○, Lauterbach●, Rother). An important interface has been established with experts in the area of electrochemistry (Eichel, Mayrhofer, Waldvogel○) and extensive analytics such as liquid and solid-state NMR or X-ray absorption and emission spectroscopy (Wiegand●, Zobel○). Fundamental engineering aspects of the production processes are being addressed from a materials basis, through reaction engineering concepts, and finally a systems process engineering perspective. The competences cover the reaction and process engineering of (bio)catalytic transformations (von der Aßen●, Jupke, Leitner, Magnus●, Mitsos, Wessling) as well as electrochemical devices (Eichel, Mechler●, Wessling).

In SRA-RACS, resilient and adaptive systems design perspective is developed. Aiming at a predictive and integrated fuel & chemical design, the developments in SRA-RACS are implemented into full process chains with the aid of predictive models linking molecular structures to performance of liquid energy carriers and chemical building blocks (von der Aßen●, Mitsos, Pischinger, Pitsch). Direct environmental impacts are determined at an early fuel design stage in order to allow for a predictive assessment of fuels, fuel blends and chemicals (Backhaus●). System Integration bases on integrated models depicting the coupling of the sectors energy, transport and chemistry (von der Aßen●, Walther), which are then extended by socio-economic and socio-political implications, specifically regarding aspects of systemic risk analysis (Arning●, Ziefle), stakeholder incentives (Walther, Venghaus●), and policy design (Venghaus●, Walther). System integration results are then combined with an environmental life-cycle assessment (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 the individual PIs, 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).

In order 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 CoE builds on the independent expertise from the Institut für Energie- und Umweltforschung Heidelberg gGmbH (ifeu). Their experts are invited to participate in the Fuel & Chemical Design Forum and critical assessments for specific case studies are commissioned. This ensures an unbiased reflection on the results providing important feedback for the continuous structuring progress of the research activities. The dissemination of the research results and public outreach will be supported by the 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.

Guidelines for section 4.5:

Describe the research programme in detail following the structure outlined in section 4.3. For each subunit of the research programme, please list the principal investigators and other key researchers and address the following points:

- specific research objectives of the subunit and its contribution to the overall objectives of the Cluster of Excellence;
- current state of research;
- individual or joint preliminary work, in case of renewal proposals: results from the previous funding period;
- work programme (approaches, methods, risks and opportunities, alternative strategies);
- if applicable: relevance of sex, gender and/or diversity dimensions, see `https://www.dfg.de/diversity_dimensions`;
- research data handling, see `https://www.dfg.de/download/pdf/foerderung/grundlagen_dfg_foerderung/forschungsdaten/forschungsdaten_checkliste_en.pdf`;
- if applicable: use of existing or planned research and/or information infrastructures;
- internal and external collaborations;
- if applicable: legal and ethical aspects of research in the subunit (cf. section 4.6.)

For each research subunit, please provide summaries of requested staff positions and funds using the tables below, and include a justification for your request in the text.

structure & page estimation:
5 subsections (SRAs): 13 pages per subsection (SRA)
SRA Summary: approx. 1 paragraph
SRA Strategy and Structure: incl. Summary max. 1-1.5 Pages
3 sub-subsections per SRA: approx. 3 pages per sub-subsection
short summary: approx. 1 paragraph
Previous work: approx. 1-1.5 pages
Objectives: approx. 0.5 pages
Work Program: approx. 1-1.5 pages
Tables: approx. 0.5 pages

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-CBFA) focuses on the conversion of carbon-based fuels in existing and future propulsion systems, both internal combustion engines (ICEs) and fuel cells. The high efficiencies and near-to-zero emissions were achieved in the current funding phase with novel bio-hybrid fuel molecules and fundamentally new combustion systems like molecularly controlled combustion systems (MCCSs), which can only be implemented in new engines and vehicles. 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 that are suitable for existing vehicles on the one hand, and at the same time gain advantages without or with software or/and hardware adaptions, 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 restricted to realization by a piston change, but not through an increased stroke. The resulting more unfavorable surface-to-volume ratio will lead to reduced efficiencies and higher hydrocarbon emissions. Therefore, we will build-up on the methodologies that we developed in The Fuel Science Center (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 for the usage in direct liquid fuel cells (DLFCs) as propulsion systems. The fuel design process will be extended to DLFCs in order to exploit the potential of a simultaneous optimization of fuel and DLFCs with novel catalytic materials.

Strategy and Structure of SRA

The SRA-CBFA explores the highly efficient and near-to-zero pollutant emission conversion of liquid energy carriers in form of hydrocarbon molecules, focusing on bio-hybrid fuels and fuel blends. Research topics include the combustion processes and the electrochemical conversion at the molecular level (CA1), as well as the associated energy conversion systems ICEs and DLFCs at the device level (CA2). In line with the holistic, integrated Fuel & Chemical Design Process (FCDP), the results contribute on the one hand to defining requirements for new fuel molecules and blends (SRA-TCP & SRA-CSP), and on the other hand, to the design and assessment of resilient and adaptive mobility systems (SRA-RACS).
FSC^2 transfers the findings on MCCSs as well as 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 efficiency combined with high energy and power densities.

Heufer

4.5.1.1 Bio-hybrid Fuel Characterization

The focus of the overarching optimization problem within the Fuel & Chemical Design Process has been on minimizing greenhouse gas emissions and the environmental impact of pollutant emissions as well as resource-efficient production. These still essential target variables are now supplemented by the compatibility of the fuels with existing powertrains opening up new research questions regarding the physico-chemical properties and requirements of bio-hybrid fuels and fuel blends in both fleet compatible thermal as well as prospective electrochemical conversion systems. Complex reaction mechanisms and molecular interactions are understood and modeled using machine learning (ML) methods in combination with intelligent sampling techniques and integrated into the established Fuel & Chemical Design Process. The in-depth understanding of the efficient energy conversion, emission formation, and molecular interaction of compatible bio-hybrid fuels is fed back into production (SRA-TCP & SRA-CSP) and contributes to the comprehensive 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][213], of rate constants [8, 9], and of 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, and handling the ever-increasing complexity of detailed models becomes challenging. 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 [214][263] and parameter estimation [263].

The highly recognized FSC-tool ChemTraYzer (CTY) (reviewed by [264, 265, 266]) performs MD simulations to find new reaction pathways and obtains accurate properties of the reactions by automated high-level quantum mechanics (QM) calculations [6, 8, 18][215, 213].

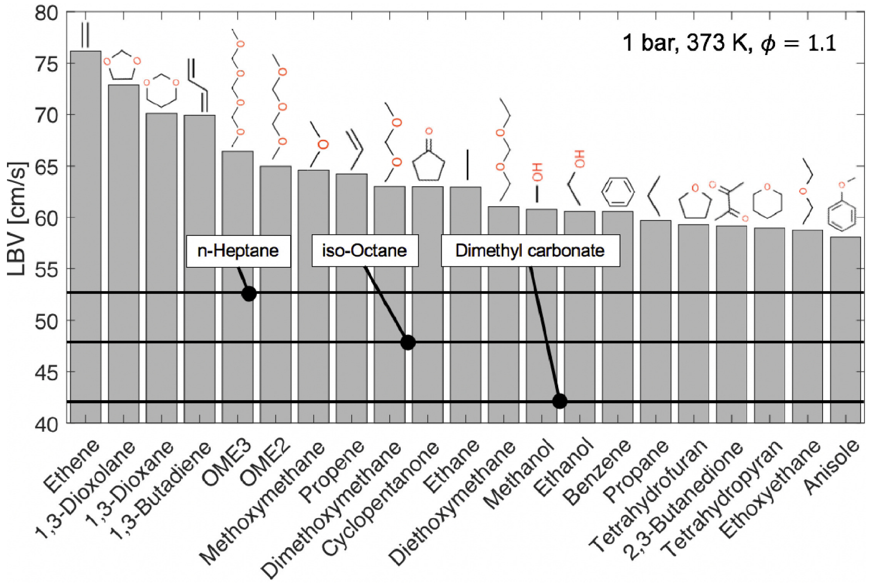

Figure 8: Ranking of fuels in the present training set with highest predicted LBVs at 373 K, 1 atm, and ϕ = 1.1. The values of n-heptane, isooctane, and dimethyl carbonate (which has the lowest value of all considered fuels) are included for comparison.[11]

However, achieving the ambitious goal of developing fleet compatible bio-hybrid fuels demands further advancements. In addition to the predictive modeling of the oxidation of various carbon-based fuels, investigating the combustion of blends becomes crucial [19]. This becomes even more challenging when hydrogen and ammonia are introduced as potential clean energy carriers. The developed kinetic models must be able to predict pollutants such as nitrogen oxides and polycyclic aromatic hydrocarbons, while also accounting for new pathways involving C-N and C-O bonds, which leads to unprecedented complexity when developing these detailed chemical kinetic models, and traditional model development methods must be amended.

Recent advances in data-driven ML, particularly in natural language processing (NLP) techniques [267, 268][20], 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 [269]. Owoyele and Pal [270] 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 [21] will be key to the further development of this method.

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, 22, 23, 4].

For the species measurements, two different laser systems are being used. The ultraviolet (UV) laser system is a single wavelength system, which excites the $\dot{O}H$ radical at 306.9 nm or 308.61 nm. By measuring the $\dot{O}H$ radical concentration, the reaction rate of the very important reaction: $\text{fuel} + \dot{O}H \Leftrightarrow \text{fuelradicals} + H_2O$, can be measured. The second laser system is an infrared (IR) laser that measures a wavenumber range of $60\,\text{cm}^{-1}$ with a time resolution of $4\,\mu$s. The currently used central wavenumber is $1740\,\text{cm}^{-1}$ and is able to measure the stretching of the carbonyl group, for example in formaldehyde [271] or alkyl formats [24] but can be exchanged by other laser modules.

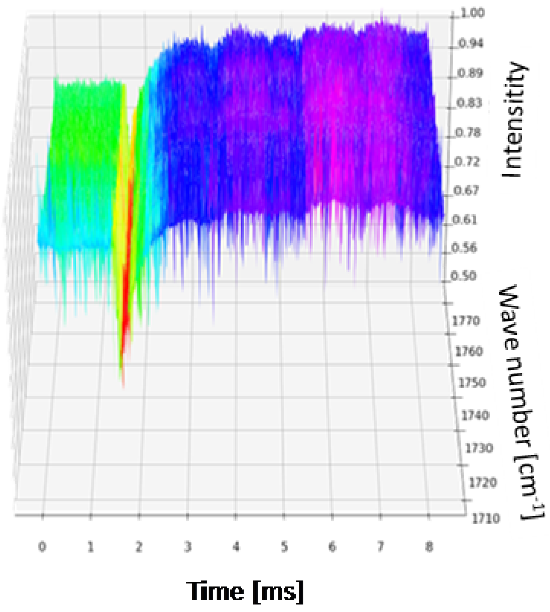

Figure 9: Measured time-resolved IR-absorption spectra during ethylformate pyrolysis (Bild austauschen)

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 mixture 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. To resolve this, species and mixture spectra could be calculated with the help of quantum mechanics and used to analyze the experimental spectrum [4, 9, 25, 26]. For the GCMS measurements, a sample needs to be taken from the reactive mixture in ST or RCM by fast opening valves (opening time: 1 ms). Currently, both systems are used separately and especially the analysis of the IR laser measurements is of challenge when several species-spectra overlap. To resolve this issue, a new analysis software is needed that uses both measurements, for GCMS and IR laser at the same time. This would give the opportunity to have advanced time resolved information about the combustion process, the pollutants formed, and the influence of different experimental conditions and molecule structures.

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 (quantification/indicators possible?), 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:(i) a new analysis tool for complex multi-component spectra using a combination of QM and MCR aided with GCMS species measurements, and (ii) a new rapid multi-sampling technique with significantly decreased sampling time to achieve high temporal resolution.

Work program

Modeling the chemical energy conversion is a critical aspect for predicting the performance of novel energy carriers and fuel blends. Conventional methods are time consuming, require high human effort, and become more and more challenging due to increasing complexity. In this context, ML-based methods offer high potential to overcome this issue by improving the model development process or even bypassing it.

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 (Iris-F1) 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.

The program will integrate various disciplines, including process modeling, environmental health & safety (EHS), and LCA, aiming to develop cleaner and more efficient energy conversion systems. Multi-disciplinery collaboration with internal and external partners will facilitate the integration of cutting-edge techniques like graph- and convolutional-neural networks for molecular property prediction.

The infrastructure in form of the High Performance Computing (HPC) platform provided by RWTH will be essential for intensive computational tasks to incorporate additional measurement techniques and advance model development.

In conclusion, this interdisciplinary research program will bridge data-driven modeling with advanced experimental investigations to advance the understanding of fuel properties, combustion processes, and electrochemical energy conversion.

4.5.1.2 Thermal Energy Conversion

Pischinger

The highly adaptive design of molecularly controlled propulsion systems is developed along a multi-stage, fleet compatible efficiency walk, which exploits the potential of bio-hybrid fuels with regard to maximum efficiency and lowest pollutant emissions within the respective level of soft- and hardware modifications to engines and exhaust gas aftertreatment systems. The opposing effect of measures to increase efficiency on pollutant emissions is further exacerbated by the restrictions imposed by fleet compatibility. For example, near-wall effects due to non-ideal surface volume ratios and the associated emissions of unburned fuel components will play a decisive role. The associated scientific questions form a connection to SRA “Ammonia Fuel Utilization” (SRA-AU), where the significance of near-wall effects is also high, due to the slow burning velocity of ammonia - even with higher degrees of freedom regarding engine design. Additional close links to SRA-AU as well as the topic of DLFCs exist with regards to material compatibility as well as the conversion of pollutant emissions in the exhaust gas aftertreatment system.

Within the Fuel & Chemical Design Process, the propulsion system design is already inherently coupled to the LCA. In the context of fleet compatible fuel as well as engine and exhaust gas aftertreatment co-optimization, the simultaneous evaluation of existing and future fuel and emission legislation as well as social acceptance plays a particularly important role (SRA-RACS).

Current State of Research and Previous Work

In FSC, molecularly controlled combustion systems were introduced, which were divided into a high-tumble (HT) and a high-swirl (HS) approach based on the main charge motion. For these approaches, dedicated combustion concepts were developed: (1) a molecular torch (MT) for the HT and (2) a molecular spark (MS) for the HS. The MT was realized by using an active pre-chamber (PC) in an HT ICE. Whereas the main chamber (MC) of the ICE was fueled with a low reactivity (LR) fuel, the PC could be 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 HS ICE with an undivided combustion chamber. In this way, the combustion process was controlled by the reactivity share and the injection timing of the fuels. The continuous development of the MCCSs yielded an increasing η_i up to a maximum of $\eta_i = 49.1\,\%$ by using a CR of CR = 19, see Figure 10a [19, 27, 28, 29, 30, 31, 32, 33]. For comparison, when using an active PC on an ICE with CR = 14, Peters et al. [272] 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 with respect to the NO_X-soot trade-off, were reduced when using the MCCS, representing near-to-zero pollutant emissions, see Figure 10b [32].

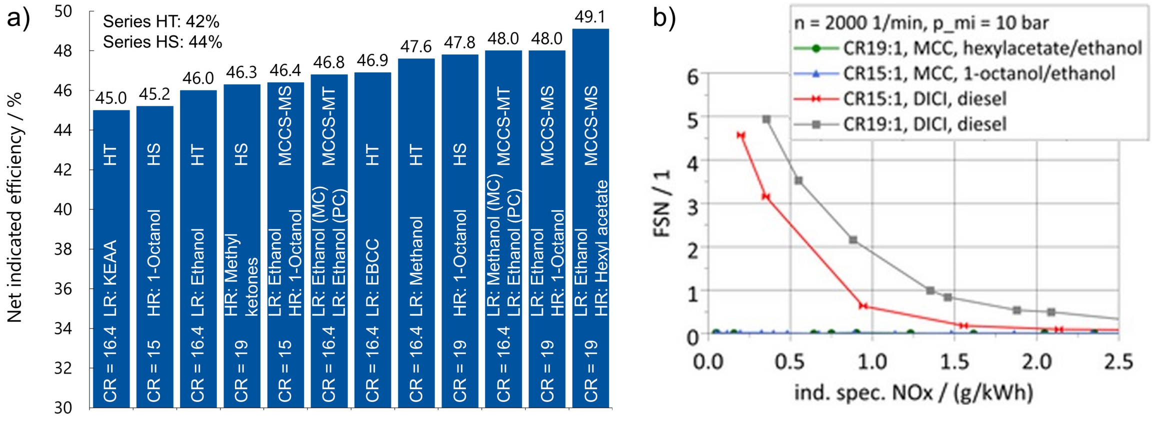

Figure 10: molecularly controlled combustion systems: a) efficiency walk; b) NO_X-soot trade-off.

The MCCSs were the core combustion concepts in FSC. Despite their experimental assessment on thermodynamic ICEs, their in-detail understanding was supported by dedicated fundamental experimental and numerical investigations.

In optical investigations on constant volume chambers (CVCs), the injection of novel bio-hybrid fuels was assessed. First, their injection plumes with respect to the penetration length, the spray cone angle, and the liquid fuel probability were examined, ensuring that the novel fuels did not indicate disadvantages over conventional fuel. Second, the ignition of LR-HR fuel combinations was assessed. Here, alternative fuels such as ethyl acetate as LR fuel and diethoxymethane as HR one were assessed. REF

Moving from a CVC to an ICE, the interaction between the injected fuels and the charge motion becomes crucial. Hence, dedicated optical investigations on an optically accessible ICE were performed. The optical results were not only used to evaluate the charge motion but also to provide a validation basis for dedicated numerical simulations of both the fuel evaporation and the mixture formation. In this way, the results of both the optical investigations and the numerical simulations provided the basis for optimizing the injection timing for the investigations on thermodynamic ICEs. REF

In case of the MT, the interaction of the PC jets with the MC charge was also important to evaluate. Both numerical simulations of the ICE 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 11. REF

Toward the end of the combustion process, the interaction of the flame with the combustion chamber walls becomes crucial because it is a source for emissions of unburned fuel, which result from the flame quenching at the combustion chamber walls. To this end, a methodology was developed to examine the resulting quench distance in optical investigations on an RCM using a dedicated quenching object, see Figure 12. The air-fuel mixture was centrally ignited inside the RCM, causing the resulting flame to propagate in parallel to the surface of the quenching object. Here, an image in the visible light spectrum was taken. Then, the flame front was extracted from the image using a post-processing code. In this way, the distance between the flame front and the surface of the quenching object, i.e., the quench distance, was determined. This evaluation methodology was also applied to coated quenching objects to assess the influence of the catalytic respectively thermal coating on the quench distance. In addition, the influence of wall coatings on the emissions was evaluated on a thermodynamic ICE, indicating

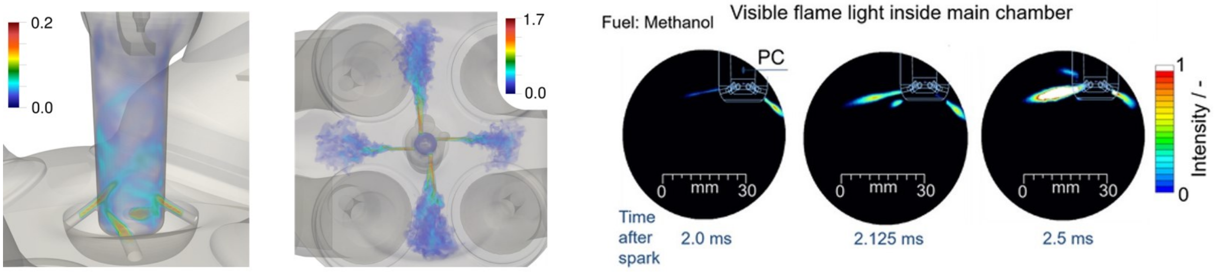

Figure 11: Numerical (left) and optical (right) investigation of pre-chamber jet ejection of the molecular torch.

that a dedicated coating enabled the reduction of both major HC species and CO. [20]

In addition to the reduction of pollutant emissions by adjusting the combustion process, dedicated exhaust gas aftertreatment systems were developed to reduce the remaining engine-out emissions by decreasing the light-off temperature of catalytic converters. In particular, a methodology to investigate the use of microwaves for the reduction of the light-off temperature was developed, revealing that catalysts performance of the materials under investigation depends not only on thermal MW-input and composition (i.e. the degree of substitution in the oxide lattice) but also on the specifics of a microwave based activation treatment in inert atmosphere. This activation treatment leads to considerably increased catalytic activity with activation energies for dry CO oxidation decreasing from 35.90 kJ/mol (pristine sample) to 23.07 kJ/mol (MW-activated sample) in the case of $La_{0.8}Sr_{0.2}CoO_3$ [34] (new paper 2024?) This approach thus offers the possibility for an efficient and adaptive low-temperature exhaust aftertreatment process.

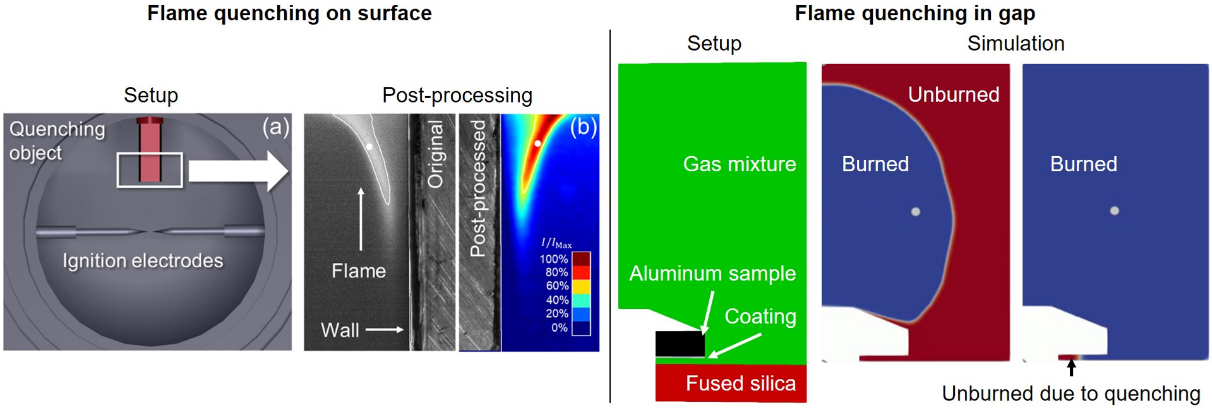

Figure 12: Left: flame quenching on (coated) quenching object in RCM [20]; right: simulation of flame quenching in (coated) gap.

Fuel blends are particularly relevant with regard to the holistic design of fleet-compatible fuels with advanced combustion properties and sustainable production. FSC has identified a number of promising fuel blends using the established FCDP.Verweis auf anderes Kapitel.

The highly knock-resistant fuel blends EBCC[1] and KEAA[2] were investigated in a thermodynamic HT ICE [19, 30]. The ketone-esters-alcohol-alkanes (KEAA) application achieved a similar η_i to 2-butanone, and the EBCC one even slightly outperformed ethanol, see Figure 10 [19, 30].

A high-reactive blend consisting of methyl ketones, was designed for HS ICEs [33]. The application of the 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.

For the fuel application in the current vehicle fleet, hydroformylated Fischer-Tropsch (HyFiT) fuels were developed and investigated. These fuels (i) used mature technologies, (ii) were com-

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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

patible with global fuel standards and elastomer materials, (iii) reduced combustion-induced emissions, such as NO_X and particulate matter (PM), and (iv) supported the transition to net-zero greenhouse gas (GHG) emissions. The investigations revealed the potential of HyFiT fuels with 20 and 40 wt % alcohol content (HyFiT-20 % & HyFiT-40 %) to replace diesel fuel in a light commercial hybrid electric vehicle. Used as drop-in fuels without any further adaptations, the HyFiT fuels reduced the engine-out PM emissions by 55 % (HyFiT-20 %) respectively 70 % (HyFiT-40 %) and the CO_2 tailpipe emissions by 3–5 % compared to diesel fuel. Adapting the calibration, in this case the exhaust gas recirculation (EGR), promises a reduction in nitrogen oxide emissions of up to 37.5 %, as shown in vehicle simulations (see Figure 13)(Quelle: HyFiT).

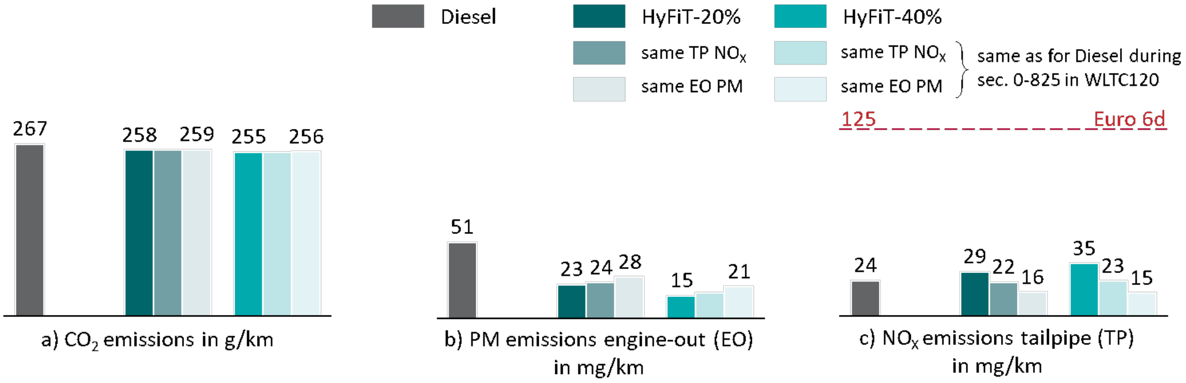

Figure 13: cumulative a) carbon dioxide (CO_2), b) particulate matter (PM) and c) NO_X emissions during WLTC120 of Diesel, HyFiT-20 % and HyFiT-40 % fuel with optimized calibration for emission reduction

Ensuring the long-term material compatibility of bio-hybrid fuels with engine, fuel cell, and infrastructure components is crucial for the successful integration of fleet compatible fuels into existing and prospective energy conversion systems. Immersion tests, as part of FSC's comprehensive fuel investigations [35, 36, 33][Quelle: HyFiT], revealed a critical increase in volume of up to 200 % for some combinations of fuels and sealing materials, particularly for molecules with both polar and non-polar functional groups and short chain-length molecules that favor diffusion processes into the sealing material [273].

Current ML algorithms, just like most experimental methods, relate to instantaneous compatibility. Long-term compatibility, on the other hand, which is becoming increasingly important against the background of sustainability and striving for longer intervals of usage, is still completely unknown.references?

Objectives

The concept of fleet compatible fuel and engine co-optimization is clustered in the multi-stage efficiency walk that transfers the efficiency walk revealed in FSC to real world applications. As a baseline, existing series production engines shall be fueled with new bio-hybrid fuels or fuel blends identified via the FCDP implemented with correspondingly stringent constraints that ensure fleet compatibility. In this way, the potential of these fuels for both the reduction of pollutant emissions and the increase of the efficiency shall be unveiled without adaptations of the engine hard- and software. In the second stage, adjustments of the calibration setting shall unlock additional potential of the bio-hybrid fuels, still without hardware adaptations. The adjustments of the calibration aim to tailor the heat release rate and to reduce the pollutant emissions for example by adapted injection or EGR and optimized exhaust gas aftertreatment strategies. In the final stage, hardware adaptations shall be considered. The advanced molecularly controlled combustion systems molecular torch and molecular spark discovered in FSC are to be implemented under the stringent, fleet compatible boundary conditions. This involves hardware adaptations such as the implementation of a piston that enables a high CR in combination with a PC and a dual-fuel injection system as well as in-cylinder coatings. Increasing the CR with fixed stroke leads to less favorable surface-to-volume ratios, making measures to reduce wall effects such as coatings more necessary.

SRA-CBFA will (i) identify bio-hybrid fuels and fuel blends that are compatible with the existing vehicle fleet, (ii) co-develop a highly adaptive molecularly controlled propulsion system design, yielding an net indicated efficiency of $\eta_\mathrm{i} > 50\,\%$ for on-road passenger cars, and (iii) enable a zero-impact emission strategy by combining the molecularly controlled propulsion system with a tailored and adaptive exhaust gas aftertreatment system, despite the restrictions of fleet compatibility fuel and limited hardware modifications.

Work program

The objectives shall be addressed through a close alignment of experiments, numerical simulations, and theory within the subtopics (i) combustion concept, (ii) exhaust gas aftertreatment, and (iii) material & device compatibility.

The MCCSs use different special-purpose, bio-hybrid fuels to enable high net indicated efficiencies with minimum emissions based on low temperature combustion with fast heat release at high CRs and strongly reduced wall heat losses. It has been demonstrated in highly optimized single-cylinder research engines (Quellen?). The challenge of fleet-compatible engine design lies in the limited degrees of freedom, particularly with respect to the base engine (peak pressure limit), crankshaft (stroke/bore ratio (s/D ratio)) and cylinder head (intake ports, charge motion, and combustion chamber access). As possible degrees of freedom remain, with increasing degree of effort, (i) the calibration and operating strategy, (ii) the ignition system, (iii) the injection system, and (iv) the piston. The latter allows for an increase of the CR, which has a positive effect on efficiency, and the application of a combustion chamber coating to reduce wall heat losses and hydrocarbon (HC) emissions.

Potential improvements by means of calibration settings are in particular, adjustments to the EGR rate, the injection strategy, boost pressure and valve timing that can be implemented in the field. Prior to experimental implementation on a single-cylinder research engine or a test vehicle, an initial assessment of potential is carried out using the vehicle simulation tool chain established in FSC. Using virtual calibration, the entire vehicle including exhaust gas aftertreatment and hybrid powertrain operation strategy will then be optimized in terms of fuel consumption and pollutant emissions (Pischinger). This allows the impact on the overall system to be integrated into the LCA (see section 4.5.5.3) at an early stage of development (e.g. ref HyFit?). Optimized injection strategies target for instance injection timing, rate and (digital) rate shaping to exploit the fuel's capability for stable lean combustion while maintaining at low pollutant emissions.The calibration of the EGR rate plays an important role in emissions behavior, particularly with regard to existing vehicles with compression-ignition combustion systems. Numerous studies have shown that a significant reduction in soot emissions can be achieved with oxygenated fuels without any adjustment to the calibration (Quellen). By increasing the EGR rate via the calibration, this effect can be used to minimize nitrogen oxide emissions as well.

The MT will be applied to the fleet compatible MCPS as retrofit ignition source (Pischinger). One challenge lies in the compact design of the pre-chamber, which has to fit into the existing spark plug bore, not only in terms of packaging, but also due to the resulting disadvantages of its effectiveness in terms of scavenging, residual gas content and turbulence level. While a passive pre-chamber may appear advantageous in terms of packaging and costs, active pre-chambers should be considered in order to be able to exploit the full potential of the MCCS. This requires adjustments to the injection system, possibly including an additional, small fuel tank or reformer.

For the introduction of the MS process into the existing vehicle fleet, the injection system must be adapted. This is conceivable, for example, via an additional port fuel injection system leading to a highly homogeneous mixture, yet a potential increase in HC emissions. Therefore, combinations with internal engine measures to reduce near-wall effects (flame quenching) such as combustion chamber coatings as well as an effective exhaust gas aftertreatment system that is particularly active in the cold start phase are especially important to consider here.

Highly knock-resistant bio-hybrid fuels and fuel blends can unlock the efficiency potential of high compression ratios. In the existing vehicle fleet, this can only be sensibly implemented by adapting the piston, as the s/D ratio is determined by the crankshaft. In terms of efficiency, an increased s/D ratio would be desirable, as the compact combustion chamber achieves a better surface to volume ratio and thus lower wall heat losses. In addition, an extended stroke improves and intensifies the charge movement. Therefore, the disadvantages of a constant s/D ratio must be counteracted here - for example, by reducing wall heat losses through combustion chamber coating (Pischinger, Heufer, Simon).

Due to the important influence of the cylinder flow field for all measures, the interaction between charge motion, fuel injection and combustion chamber walls has to be understood in detail. CFD-based optimization methods developed and established in FSC are used for this purpose. The optimization process, based on a Kriging model (Quelle?), includes the shape parametrization of the cylinder head (including intake ports), pre-chamber, and piston geometry. Here too, special attention is paid to the near-wall effects and the precise depiction of the combustion chamber crevices. Besides the geometry, the combination of fuels and multiple fuel-injection parameters are determined with the ultimate objective of high efficiency and low emissions (Schröder)(Quellen?).

Associated with these strategies are challenges requiring a principal understanding of the relevant physical and chemical processes. That for, experiments will be performed under well-defined engine-relevant conditions in a constant pressure flow (CPF) vessel and a single cylinder engine (SCE) with optical access (Boxx[3], Pischinger). The goal of these experiments is to obtain accurate, high precision near-wall measurements of temperature and species concentrations at engine-relevant conditions with spatial resolution significantly smaller than that of the quench distance. The extreme technical challenge of acquiring such data at engine-relevant conditions will be addressed through the development of an innovative, 2D measurement system based on femtosecond Coherent Anti-Stokes Raman Spectroscopy (fs-CARS).

Coherent Anti-Stokes Raman Spectroscopy (CARS) is a well-developed technique for accurate, high-precision measurement of temperature and major species concentrations in turbulent flames. It requires only minimal optical access and generates background-free measurements with sufficiently strong signal for single-shot measurements. A strong non-resonant signal originating from in-cylinder hydrocarbon molecules (i.e. fuel or residual lubricants) however, limits its viability for high precision near-wall measurements in an optical engine. This limitation may be overcome through the use of femtosecond duration laser excitation, which enables one to probe excited coherences shortly after the excitation pulse and thereby eliminate the problematic non-resonant signal. Furthermore, the high peak power enables two-dimensional fs-CARS imaging for simultaneous temperature and concentration measurements with high accuracy, typically with less than a 3 % error. Combining fs-CARS and fs laser-induced plasma generation allows for reliable detection of N_2 and O_2 in addition to product gases such as CO, CO_2, H_2O, and NO_X in turbulent conditions.

This exciting new measurement capability, particularly in combination with well-developed techniques such as laser-induced fluorescence (LIF), Raman scattering spectroscopy, chemiluminescence imaging will significantly enhance understanding of piston wall effects and flame-wall interactions with catalytic and thermal coatings under real engine conditions.

Unfavorable surface to volume ratio in retrofit solutions increases the risk of pollutant emissions such as unburned hydrocarbons under real conditions, especially during cold starts. In addition to exhaust gas aftertreatment measures for lean-burn processes to reduce nitrogen oxide emissions (see section 4.5.2.3), particular attention should therefore be paid to rapid warm-up and early conversion at low exhaust gas and ambient temperatures. To this end, the fundamental findings on microwave-activated exhaust gas catalysis (Simon, [34] (new paper 2024?)) and 3D-printed catalyst carriers (Wessling, Quelle linkhorst/CVT) are to be combined into adaptive retrofit concepts and tested under realistic conditions on the laboratory gas test bench (Pischinger). The experimental investigations are accompanied by multi-scale simulations for a deep understanding of the underlying physico-chemical processes (Khetan[4]).

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). That for, material and

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

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

device compatibility of new fuel candidates have to be investigated both numerically and experimentally. For the experimental investigation of long-term compatibility of these fuels without falsifying the significance of the results, new accelerated tests have to be developed (Schmitz). To facilitate the process for the evaluation of long-term behaviour of static and dynamic seals and low-viscosity liquids with both non-polar and polar components, the comprehensive data base gained by accelerated testing is utilized for a machine learning classification based on the molecular character of fuels and sealing materials for the prediction of compatibility and elastohydrodynamic lubrication (EHL). Since the simulation of long-term wear phenomena is related to high computational costs, fast-EHL approaches, which were developed at Institute for Fluid Power Drives and Systems (ifas), are to be integrated. Accompanying and validating the new accelerated test procedures as well as the new ML methodology, long-term immersion tests, tribological experiments and determination of fluid physical properties with the measurement infrastructure already established in FSC (automated immersion test bench, drop-shape analyzer, densimeter, tensiometer, viscometer) are conducted.

Mechler

4.5.1.3 Carbon-based Fuel Cells

Non-H_2 fuel cells or DLFCs show great potential as energy conversion systems with zero or near-to-zero environmental impact. DLFCs share a variety of advantages to the currently more prominent hydrogen fuels cells: The liquid fuels have higher energy densities than compressed hydrogen and are easier to handle. In fact, they could be distributed by the existing fuel infrastructure and allow simpler fuel handling in the refueling stations as well as in the fuel cell system. Their role as hydrogen carriers in a future carbon-hydrogen economy makes them interesting for direct use in energy converting technologies.

Currently, methanol and ethanol are the most prominent DLFC candidates. In the research field, however, there is a large variety of possible fuels that can be converted for electricity generation. Also, first reports have shown that some fuel cells can tolerate different fuels simultaneously, allowing flexible fuel use, making them highly adaptable. For their further development, new materials in terms of 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 a broad range of applicability. The development of non- or low-noble metal-based catalysts for the anode as well as fuel-resistant cathodes and improved membranes is supposed to lower the overall costs of DLFCs. We will cover 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 the flexible use of different fuels as well as blends thereof to allow for highly adaptive and resilient systems. Also the use of new fuels from the FCDP within FSC^2 will be considered. 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.

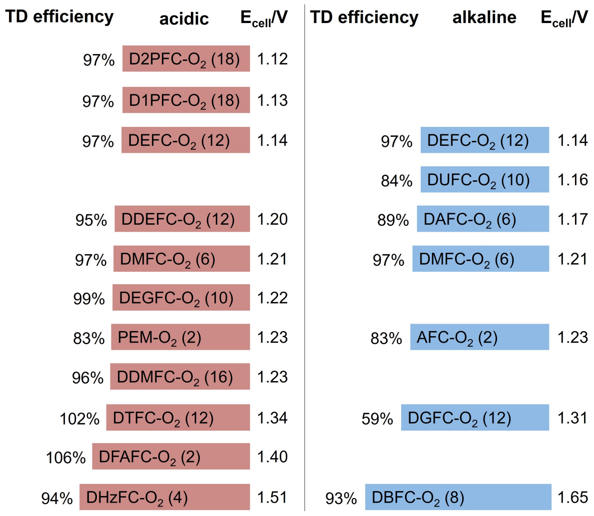

Figure 14: ***Illustration of most prominent DLFCs reported in literature, including direct 2-propanol fuel cell (D2PFC),direct 1-propanol fuel cell (D1PFC), direct ethanol fuel cell (DEFC), direct urea fuel cell (DUFC), direct ammonia fuel cell (DAFC), direct dimethylether fuel cell (DDEFC), direct methanol fuel cell (DMFC), direct ethylene glycol fuel cell (DEGFC), direct dimethoxymethane fuel cell (DDMFC), direct glycerol fuel cell (DGFC), direct trioxane fuel cell (DTFC), direct formic acid fuel cell (DFAFC), direct hydrazine fuel cell (DHzFC), and direct borohydride fuel cell (DBFC). The numbers in brackets indicate the transferred number of electrons. The maximum possible efficiency is calculated from thermodynamic data.***

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 [274, 275]. 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). Furthermore, the use of DLFCs for mobile applications was analyzed and especially for heavy duty as well as remote applications the high power density and easy storability of liquid fuels can outperform conventional H_2 fuel cells (Figure DLFC_Applications, Pischinger).

A common problem for all molecules containing at least two C-atoms is the difficulty of breaking the C-C bond and, if achieved, the poisoning of the often Pt-based catalysts by intermediates like CO [275, 276]. The problem of poisoning could be overcome by utilizing non-noble metal catalysts, that are less sensitive for the adsorption of such intermediates and furthermore significantly decrease the costs of DLFCs. For instance, carbon-based catalysts on the cathode and transition-metal based catalysts on the anode are promising alternatives [277, 278, 279]. The FSC^2 clusters vast experience in (fuel cell) catalyst development and characterization. For instance, we have studied non-noble metal and hybrid catalysts for fuel cells [216, 217, 218, 219, 220] (Mechler, Mayrhofer) as well as [...] (Palkovits). Also the degradation of electrochemical systems has been studied in-depth with modern technologies such as in-operando mass

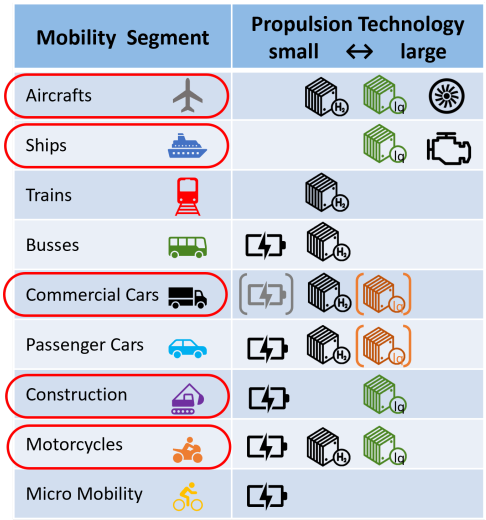

Figure 15: Applicability analysis of selected DLFCs for various mobile applications.

spectrometry [221, 222, 223, 224] (Mechler, Mayrhofer) as well as magnetic resonance imaging (MRI) [225, 226], in-operando X-ray computed tomography (XCT) [227], and 3D transmission electron microscopy (TEM) [228, 229] (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 [280], and (ii) fuel blends can even have advantages over single fuel feeds in terms of performance and cross over [281]. For this, catalyst materials that are fuel flexible need to be found, while within the FCDP fuels need to be tailored for optimal interaction.

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 built on our capacities in the field of […] (Khetan) Furthermore, a tailored fuel design should not only 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 [37] and process screening [38, 39], as well as integrated product and process design [40] (Mitsos). These approaches can be extended and applied to the application case of DLFCs. Moreover, we have experience in the modeling of electrochemical systems [41, 42] as well as in optimal design and operation [42], even applied to fuel cells [230]. 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 [43].

Another significant challenge limiting the viability of DLFCs today is the high permeability of fuels through the membranes, which leads to reduced power output [282]. Surface and material modifications, and substitution of perfluorosulfonic acids (PFSAs) by hydrocarbon membranes, have shown to increase performance [282][231]. Interestingly, larger fuel molecules, such as ethanol or ethylene glycol, as well as fuel mixtures can lead to decreased permeabilities [282, 281], again highlighting the potentials that lie within a tailored fuel design. For anion exchange membranes (AEMs), the stability and conductivity still has to be improved for a successful implementation in real devices [44][283]. Additionally, the catalyst-membrane interface needs improvement in order to reduce overpotentials [284]. Alternatively, a bipolar membranes (BPMs) in forward bias can be used to operate anode and cathode in different environments. Research in this field is still in its infancy, but recent development in interface engineering of the bipolar junction opens the pathway towards application in fuel cells [285, 286]. Within FSC^2 extensive background in membrane formation and characterization is available. For instance, studies include the modification of PFSAs-based cation-exchange membranes (CEMs) membranes to reduce methanol crossover [232, 233], hydrocarbon-based PFSAs substitutes [231], and micropatterning to increase the catalyst utilization at the catalyst-membrane interface [45]. Additionally, Wessling et al. have developed AEMs for direct methanol fuel cells [44, 46]. 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 [47, 48], asymmetric BPMs were prepared for increased selectivity [49, 50] and modelled [51].

Hier könnte die SOFC-Einführung stehen

Last but not least, for some applications microbial fuel cells (MBFCs) are an interesting 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 [287, 288]. 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 [234, 235] (Lauterbach) and collaboration with cooperation partners for MDH-design [288] , 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. 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 optimized 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-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. While low-temperature systems are investigated mainly for mobile applications, high temperature systems can be advantageous for stationary applications. They are furthermore known for a large fuel flexibility due to internal reformation processes. We will study the impact of fuel blends or alternating fuel compositions on the long-term stability. This will be monitored by online electrochemical impedance spectroscopy (EIS) as well as product detection, which is furthermore needed for a tailored aftergas treatment. Regeneration strategies by short-term reverse operation will be investigated to define optimized operation protocols, minimizing degradation rates. We will hence investigate the fuel flexibility of state-of-the-art systems and the impact on operation as well as material stability (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 [289]. 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-CBFA

Table 4.5.1.1: Proposed Staff in SRA-CBFA

	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

Continued on next page

(Continued)

	2026	2027	2028	2029	2030	2031	2032
Postdoctoral researchers	0	0	0	0	0	0	0
Doctoral researchers	10.5	10.5	10.5	10.5	10.5	10.5	10.5
Other staff	0	0	0	0	0	0	0

Table 4.5.1.2: Funding Request for SRA-CBFA

	2026	2027	2028	2029	2030	2031	2032
Funding category	**Totals per year in thousand euros**						
Staff (Total for 4.5.1)	800	824	849	874	900	927	955
Direct project costs (excluding staff)	315	167	205	105	105	105	105
Total instrumentation < €150,000	0	197	50	0	55	0	0
Total instrumentation > €150,000	156	0	0	0	0	0	0
Femtosecond Optical Parametric Amplifier	156						

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. 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.

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-AU) develops clean systems for thermochemical and electrochemical conversion of ammonia (NH_3). The utilization of NH_3 in internal combustion engines (ICEs) and high- and low-temperature fuel cells for marine and stationary applications is highly promising in the development of carbon-neutral energy systems. However, several significant NH_3-specific challenges remain to be resolved. The low reactivity and high fuel-nitrogen content can lead to unstable combustion, low efficiency, emissions of NO_x and N_2O, and NH_3 slip for ICEs. Reactivity enhancement, tailored mixing and combustion concepts, as well as catalytic and thermal cylinder coatings will be explored from fundamental aspects to improve the efficiency of NH_3 engines and reduce 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 and proton conductors as well as poisoning and degradation mechanisms will be investigated to resolve these issues. To address the critical aftertreatment of the complex exhaust gas mixtures from both ICEs and fuels cells, catalysts for coupled DeNO$_x$-SCR and N_2O decomposition, as well as N_2O reduction by NH_3 will be developed using a combination of experimental and numerical methods.

Strategy and Structure of SRA

H_2-based energy carriers, such as molecular H_2 and NH_3, will play a special role in future carbon-neutral energy systems delete: as they can eliminate CO_2 emissions throughout the entire value chain. H_2 has a very low energy density and very high diffusivity, which make it difficult to transport and store, thereby, significantly affecting the overall efficiency [290]. In contrast, NH_3 can be liquefied under moderate pressures, which makes it well-suited for easy and inexpensive long-distance transport and long-term storage [291]. Also, its production is well understood and can be carbon neutral if based on renewable energy [292]. NH_3 can be reformed to H_2 and used in ICEs or PEM fuel cells. However, especially for the latter, the reformed gases require purification to remove traces of NH_3 and other catalyst poisons. Hence, while NH_3's toxicity limits its use to well-controlled environments, direct thermochemical and electrochemical energy conversion in ICEs and fuel cells is of high interest [293].

Since NH_3 possesses unique thermodynamic and combustion properties differing significantly from those of conventional fuels, distinct challenges arise for NH_3 engines, such as incomplete and unstable combustion and nitrogen-containing emissions. In particular, NH_3 slip and N_2O emissions are problematic, the former because of NH_3's toxicity and the latter because of the particularly high global warming potential of N_2O. To mitigate such issues, novel injection methods and combustion concepts based on molecular torch (MT) and in-cylinder staging will

be explored in combination with reactivity tailoring by partial onboard or in-engine NH_3 reforming. Therefore, the SRA-AU will exploit all degrees of freedom to develop novel NH_3 engines, in contrast to the SRA-CBFA, which focuses on modifying existing engine systems.
Compared with H_2 proton exchange membrane fuel cells (PEMFCs), direct ammonia fuel cells (DAFCs) have the advantage of utilizing NH_3 without external pre-reforming by either catalytically converting NH_3 directly in low-temperature fuel cells or by internally reforming NH_3 to N_2 and H_2 at high temperatures in solid oxide fuel cells (SOFCs). For low temperature DAFC, efficiency is a challenge, but there is great potential with new catalyst materials for ammonia oxidation reaction (AOR) and oxygen reduction reaction (ORR), as well as with improved anion exchange membranes (AEM). For direct NH_3 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 proton-conducting ceramic electrolytes (protonic conducting fuel cell, PCFC). Both direct SOFC and PCFC concepts will be considered here.

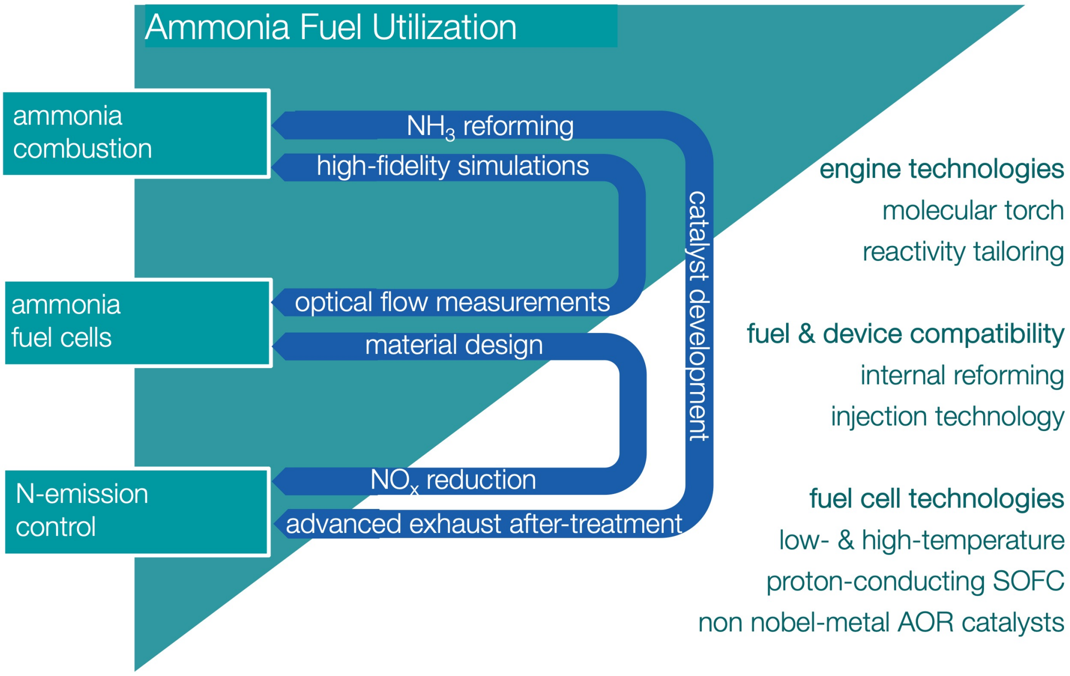

Figure 16: Structure of Strategic Research Area (SRA) "Ammonia Fuel Utilization".

The structure of this SRA is shown in Fig. 16. 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, including studies on flame speed boosting by NH_3 reforming, NH_3-H_2 blends injection, and catalytic ignition in pre-chambers. The sub-SRA "Ammonia Fuel Cells" focuses on increasing NH_3 fuel cells' efficiency and durability by identifying novel materials, such as AOR catalysts, poison-resistant cathodes, advanced proton conductors, and alkaline membranes. The sub-SRA "N-emission control" addresses the exhaust gas after-treatment for NH_3 engines and SOFC fuel cells by developing advanced catalysts and technologies capable of handling wide variations in exhaust composition, and have high solvothermal stability. The challenges of enhancing efficiency and reducing emissions in thermochemical and electrochemical NH_3 conversion will be addressed through strong interactions in FSC^2, not only within and but also outside of the SRA-AU. For example, strong connections to SRA-CBFA exist in the investigations of flame-wall interactions, emission control, and material compatibility. In addition, the strong connection with SRA-RACS will allow the consideration of efficiency, resilience, adaptability, and environmental sustainability during the development of NH_3 fuel utilization technologies.

Pitsch

4.5.2.1 Ammonia Combustion

This sub-SRA focuses on two major tasks: enhancing the combustion process in NH_3 engines and reducing the engine-out emissions. In the first project phase, we successfully developed lean-burn bio-hybrid fuel concepts using the MT ignition strategies, and catalytic and thermal coatings to enhance the 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 co-fuel enhancing reactivity and supporting 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 for heavy-duty engines. The advantages of methanol are related to a combination of outstanding knock resistance with high burning velocities [52]. 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 causes NH_3 slip [294]. 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 [295, 296], cetane boosters [297], or H_2 [298, 299, 300]. 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 [301]. A 10% rate of NH_3 reforming, for instance, was found to enhance the engine's range of stable operating conditions significantly [302]. On the other hand, H_2-rich blends tend to increase NO_x and N_2O emissions [302]. 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 [53, 54], 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 [291]. 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, is poorly understood due to NH_3's unique physical properties [298]. 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 non-linear turbulence-flame interactions, as well as the complex flame-wall interactions and formation of nitrogen-containing pollutants [303, 304].

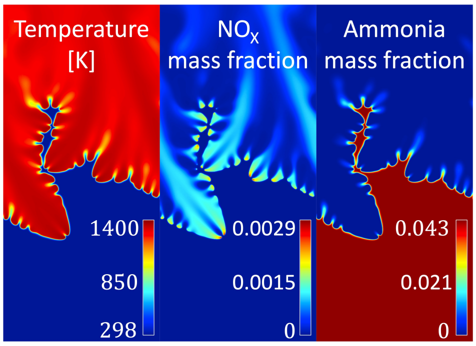

Figure 17: ***DNS of laminar NH_3/H_2/air flame with 40 mol-% H_2 showing intrinsic flame instabilities without which the flame would appear as a horizontal line.***

In our prior 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 the laminar burning velocities of NH_3/air flames under microgravity conditions in drop tower experiments [55]. Also, a new chemical kinetic model has been developed [56], and a comprehensive evaluation of 16 recent NH_3 combustion kinetic models has been performed based on an extensive experimental data set for NH_3 and NH_3/H_2 combustion [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) in Fig. 17. In addition, the already established research facilities in the project's first phase provide a powerful toolset for investigating NH_3-based combustion. These include the thermodynamic and optical engines for performance, efficiency, and emission characteristics [27, 28, 32], femtosecond two-photon laser-induced fluorescence (LIF) for temporally-resolved measurements of flame structure and dynamics [57, 58], catalytical in-cylinder coating for reducing flame quenching distance and incomplete combustion [59], transparent nozzle setup for measurements of nozzle-internal flow phenomena [60], and adaptive-mesh simulation tools for highly accurate numerical investigations of fuel sprays, flash boiling, and engine combustion [61, 62].

Objectives

The overall objective of the sub-SRA “Ammonia Combustion” is to enable heavy-duty NH_3 engines with stable combustion, high thermal efficiencies, and near-zero emissions. This will be achieved through MT using catalytic surfaces, controlled heating, and high-reactivity bio-hybrid fuels as ignition accelerators. Additional strategies include partial NH_3-reforming using highly active and selective catalysts to provide on-demand $NH_3/H_2/N_2$ mixtures, in-cylinder combustion staging with tailored stratification to suppress nitrogen oxides formation, and knowledge-based triggering of intrinsic flame instabilities to increase combustion speed, stability, and efficiency.

Pollutant mitigation requires a systematic device and process design, which must be based on a quantitative description of the interacting processes of injection, mixing, and combustion. Thus, predictive injection and combustion models will be developed for the considered advanced NH_3 engine concepts to enable computational design. High-fidelity reactive computational fluid dynamics simulations will be used based on the computational infrastructure developed during the first project phase to explore and develop novel mixing and injection strategies. Experiments in optical engines and high-pressure vessels using laser-diagnostic measurements will be performed, including newly developed techniques for quantitatively providing radical concentrations to elucidate the flame structure and the formation mechanisms of nitrogen-containing pollutants at engine-relevant conditions. Furthermore, strategies for increasing burning speeds by tailoring intrinsic flame instabilities will be developed based on high-pressure experiments and DNSs.

Delete above and use the following objectives: The overall objective of the sub-SRA “Ammonia Combustion” is to enable heavy-duty NH_3 engines with stable combustion, high thermal efficiencies, and near-zero emissions. For this objective, it is essential to develop NH_3-specific engine concepts, including the partial NH_3-reforming using highly active and selective catalysts to provide on-demand $NH_3/H_2/N_2$ mixtures, the advanced MT using catalytic surfaces and controlled heating, knowledge-based triggering of intrinsic flame instabilities to increase combustion speed, and in-cylinder combustion staging with tailored stratification to suppress fuel slip and nitrogen oxides formation, and increase efficiency. Therefore, a specific focus shall be placed on the quantitative characterization and modeling of the interacting individual processes of reforming, injection, mixing, and combustion. Based on the resulting knowledge and numerical models, we aim to develop and assess novel NH_3 engines using computational design and system-level experiments.

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 utilizing on-demand reformed H_2 or high-reactivity bio-hybrid fuels as ignition accelerators will be considered, such as enhanced MT with catalytic surfaces and active heating, enabling pre-chamber auto-ignition without a spark plug and reducing pre-chamber volume and efficiency losses, as well as targeted in-cylinder staging with novel high-pressure injection strategies for NH_3-H_2 blends, as illustrated in Fig. 18. Catalytic NH_3 reforming, either prior to or during combustion will be investigated (Palkovits), which is central to 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, building on our preliminary work [59] (Simon). 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.

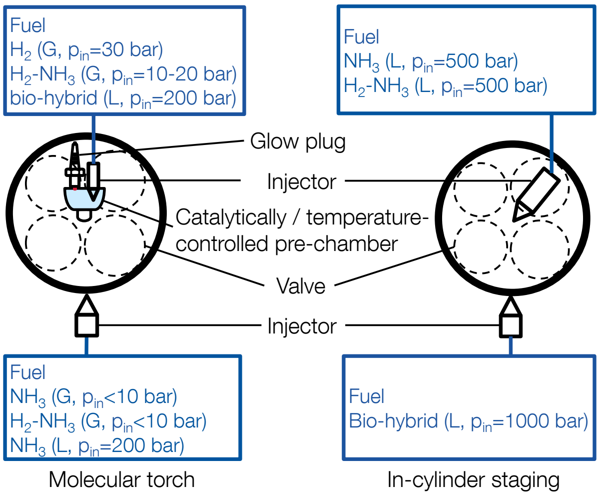

Figure 18: Ammonia engine concepts. 'L' stands for liquid, 'G' for gaseous, and 'p_{in}' for injection pressure.

For the (partially) premixed combustion concepts of MT, 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 and spatially and temporally highly resolved DNS based on a hierarchical approach (Pitsch). A multifunctional high-pressure burner facility (MHBF) will be employed to examine the effects of turbulence, flame intrinsic instabilities, pollutant formation, and their interactions in turbulent jet flames. Various combustion configurations, including premixed, partially premixed, and diffusion flames of NH_3, H_2, and bio-hybrid fuels, will be characterized in the turbulent compression reactor (TCR). 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, which will be quantitatively characterized using the TCR and DNS, focusing on the intricate interplay of mixing, auto-ignition, and flame propagation with turbulence and flame stretching in the MT concept. Further, DNS will also 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. The flame-wall interactions will be investigated jointly with the SRA-CBFA. These DNS will enable the development of high-fidelity large eddy simulation (LES) models for computational design and optimization at both device and system levels. In addition, 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.

The in-cylinder staging concept with various fuel injection strategies enables diffusion and staged combustion, potentially avoiding flame wall quenching and achieving high efficiency with low NH_3 slip. However, it presents additional challenges related to injection and mixing. 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 under feasible 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). Targeted engine operation conditions will be investigated, considering the non-linear behaviors of the complex processes, such as the temperature and pressure dependency of intrinsic instability and flash boiling, turbulence interactions with MT, and the effects of mixing and flame dynamics on pollutant formation. Computational design using high-fidelity LES and optimization approaches is necessary to effectively achieve the global optimization of the entire combustion system (Schröder). The complex injection of NH_3-H_2 blends 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.

4.5.2.2 Ammonia Fuel Cells

Mechler/
Eichel

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 is reformed 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 [305] and high temperature applications [306]. 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 [306]. Here, aftertreatment is necessary to remove NO_x as well as unprocessed NH_3. Alternatively, solid proton conducting fuel cells (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 [307, 308, 309], this also causes new challenges, for instance in developing the right catalyst to decompose ammonia at those lower temperatures [310, 311]. Typical materials for SPCFC electrolytes are yttrium-doped barium zirconate (BZY), yttrium-doped barium cerate (BCY) and yttrium-doped barium zirconate-cerate (BCZY) [307, 312]. Further doping with Yb improves the stability even more [308, 309, 313]. Within the cluster, we combine extensive experience in the field of material and cell development for SOFCs, both in fuel cell and electrolysis mode [236, 237, 238, 239, 240] (Eichel) with competences in the operation of fuel cell test benches [241] as well as fuel cell simulation addressing system performance, locally resolved electrochemical cell behavior, and mechanical stress distribution within the different cell materials [242, 243, 244] (Pischinger). First SPCFC separators have been developed with promising results at 600 °C [245] (Fig. 19), and under NH_3-operation [246]. 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 [314, 315, 316, 317, 318]. 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 [319, 320, 321, 322, 323, 324, 325]. 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 [319, 325, 326]. 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 explored previously by the applicants and was successfully applied in H_2 fuel cells [218, 220, 219] (Mechler). Further experience exists for the development and characterization of various non- or low-noble metal catalysts for energy conversion applications [247]. In preliminary studies, Ni- and Ni-Cu-hydroxides were investigated as catalysts

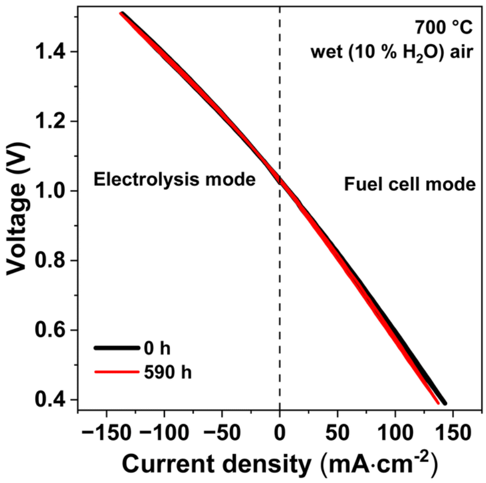

Figure 19: iV curves before and after 590 h in electrolysis operation of an electrolyte supported PNO/DNSYYb/Ni-BZY cell, showing the possibility of stable operation of SPCFCs.

for 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. 20). Furthermore, the search for anion exchange membranes (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 [63, 64, 65, 66, 67] (Schröder).

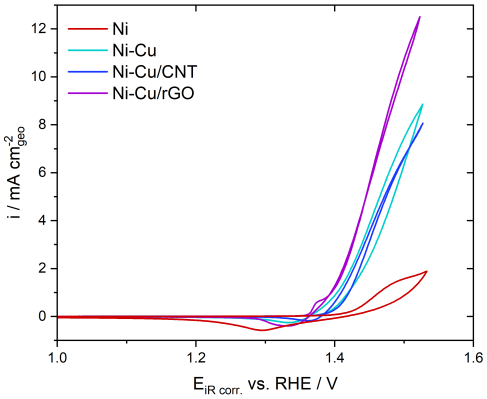

Figure 20: Rotating disc electrode measurements in 1 M KOH + 0.5 M NH_4OH for Ni- and Ni-Cu-hydroxides and the impact of supporting them on CNTs and rGO.

Objectives

DAFCs are identified as potentially highly efficient technologies 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 than GDC. 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 SOFCsis 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 Spectroscop (FTIR) and Non-Dispersive Infrared (NDIR) sensors (Pischinger).

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. also SRA CBFA, 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 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 using the Chair of Fluid Mechanics and Institute of Aerodynamics (AIA) simulation framework and micro-particle image velocimetry (PIV) experiments for volumetric flow field measurements of narrow channels and channel structures, as well as experimental analysis of the interaction of gas bubbles and fluid flow in narrow channels (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 studies open the possibility to optimize reaction conditions within short time-frames (Mitsos). Studies of economic viability and the possibility for integration into a future hydrogen economy are addressed in SRA RACS.

4.5.2.3 N-emission Control

Khetan

While commercially available exhaust after-treatment system (EATS)s can deal well with NO_x, reducing the unusually large NH_3-slip from incomplete NH_3 combustion and N_2O decomposition 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 unburned NH_3 from the other exhaust gas constituents. In addition, we will explore the use of catalytic reformers for decomposing the unburned NH_3 into N_2 and H_2. The heat generated by oxidizing H_2 to H_2O can be harnessed for raising the subsequent N_2O decomposition. To address the most difficult challenge of N_2O decomposition itself, we will develop new catalyst materials with no or low-precious metal content that can perform coupled NO_x+N_2O decomposition at lower temperatures, are capable of handling wide variations in exhaust composition, and have high solvothermal stability. We will also explore unconventional methods like microwave (MW) activation, which have shown promise in aiding heterogeneous catalysis reactions but have yet to be employed for N_2O decomposition. To achieve this, we will identify promising catalyst materials that can be "activated" under MW irradiation, and develop the corresponding after-treatment test benches. The rational design of such catalytic materials needs a fundamental understanding of the "in-operando" structure of the catalytic interfaces and the respective reaction mechanisms. We will address these challenges by developing new setups for spectroscopic operando monitoring of reaction intermediates and accelerated reactive MD simulations.

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 [68, 69, 70, 59, 71]. 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, where they also show high NH_3 storage capacity [71, 72, 73, 74][248]. 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 [72, 73, 74] [248]. However, these catalysts are mostly inactive for N_2O decomposition at such low temperatures. Ours [69, 70] and others' [327, 328] previous work indicates that the efficient decomposition of N_2O is facilitated only above 450 °C.

The best known N_2O decomposition catalysts are comprised mainly of precious metals [329, 330, 331]. 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[332, 333]. These conditions also include the inhibitory effects of O_2, NO_x, and H_2O [334, 335, 336], which are poorly understood. In addition to N_2O decomposition, it is also essential to deal with unburned NH_3. Transient combustion in an ICE exhibits disparate NH_3/NO ratios, with reported values greater than 1 **citeOthers-doi:10.3389/fmech.2020.00043, doi:10.1016/j.rser.2023.113631, doi:10.1016/j.fuel.2023.130496**. Conventionally, NH_3 slip catalysts utilized in automotive applications also form secondary NO and N_2O, thus posing significant challenges for achieving near-zero emissions. Thus, further reforming of NH_3 into N_2 and H_2 with high selectivity is both sensible and necessary.

We have previously identified universal descriptors of catalytic activity in doped oxides [249] and rationalized the effect of strong metal/support interactions [250, 251]. Recently, we employed the first-principles-based energetic span model (ESM) to analyze N_2O decomposition activity on pure and hybrid catalysts **citeClusterdoi:10.1016/j.cattod.2024.114892**. We reported the first Brønsted-Evans-Polanyi relations for N_2O decomposition, NO dissociation, and NO+O recombination, all of which enabled estimation of the turnover frequency (TOF), as shown in Fig. 21. Our work revealed excellent opportunities for enhancing N_2O decomposition by exploiting weak correlations between intermediates' adsorption free energies. and also captured quite well the inhibitory effects of NO on N_2O decomposition. Nevertheless, the operando surface of the catalyst has multiple 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 to enabling MW-stimulated catalysis for shortening the cold-start phase, we recently introduced an MW-assisted heterogeneous catalysis setup [34]. Using CO oxidation as a model reaction, this effort not only achieved enhanced conversion rates but also highlighted the critical importance of several aspects concerning the catalyst temperature distribution, thermal runaway, hotspot formation, particle size effects, as well as gas flow and system design, which will be useful for the development of the envisioned EATS for ammonia conversion devices.

Objectives

The overall goal of this sub-project is to develop an innovative and integrated EATSs for NH_3 combustion comprising of no or low precious metal catalysts that are functional at lower temperatures, capable of handling wide variations in exhaust composition, and have high solvothermal stability. Our first objective is the development of an 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

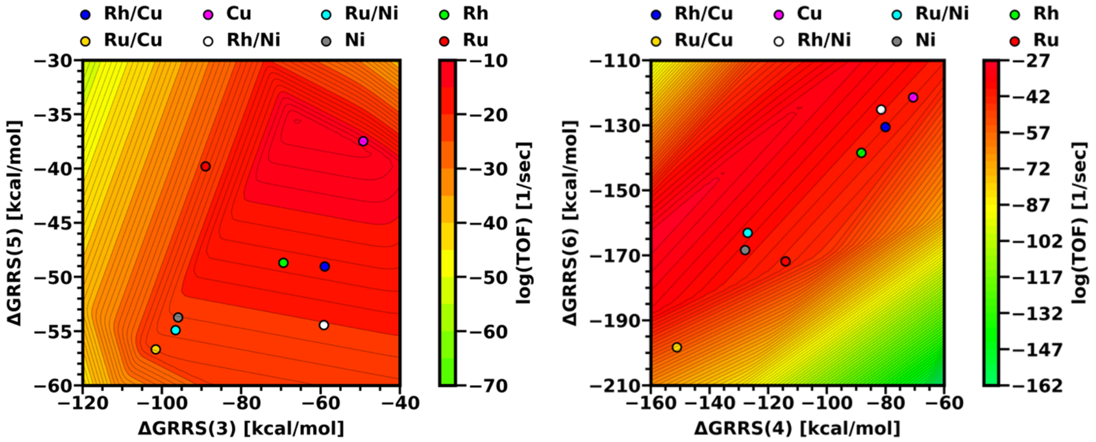

Figure 21: TOF activity maps from our work citeClusterdoi:10.1016/j.cattod.2024.114892 showing the predicted performance of various catalysts (left) in the absence of NO, and (right) in its presence. The presence of NO leads to a significant overall drop in TOF.

EATS. Our 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 **citePIdoi:10.1039/C2EE02865** 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_3reforming, and thus offer good starting points for developing a noble-metal-free system **citeOthersdoi:10.1016/j.ijhydene.2020.04.007, doi:10.1016/j.apsusc.2019.01.269, doi:10.1016/j.nanoen.2022.106929**. 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 H_2 to assist exhaust gas after-treatment via H_2-SCR [337, 338] will also be investigated.

In parallel, we will chcracterize NH_3 storage materials to enable an innovative circular capture and release process. Various material classes such as metal-halides **citeOthersdoi:10.1016/j.ijhydene.2020.01.145** and Metal-Organic-Frameworks (MOF) **citeOthersdoi:10.1002/anie.201808316** will be explored for their NH_3 storage capacity, including zeolites **citePIdoi:10.1016/j.snb.2016.05.164** [252] from our previous work. Going beyond thermally triggered release of stored NH_3, we will build upon our previous work **citePIdoi:10.1007/s11244-016-0605-z** and develop a novel strategy for triggering NH_3 release much more quickly and energy-efficiently by applying MW excitation. This work of the MW-induced release with generate strong synergies with the project “Microwave enabled ICCU”, which is part of SRA “Translational Catalytic Processes”.

For coupled DeNO$_x$-SCR with unburned NH_3 and N_2O decomposition, we will develop transition metal-promoted zeolite catalysts, such as in our recently shown direct methane partial oxidation [75]. These catalysts will be tested in conventional EATS test benches to test 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 new strategies 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 get 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 [339, 340], 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 material functionality by using non-parametric techniques such as symbolic regression or compressed sensing [341]., which can yield rapidly calculable descriptors of catalytic performance for material screening without resorting to expensive large-scale simulations.

These efforts will be complimented by spectroscopic operando monitoring of reaction intermediates and products at the catalysts' surfaces using in-situ DRIFTS, impedance, and mass spectrometry, for accurate quantification of the various NH_3-combustion 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 [342, 343] 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 interatomic potentials [344, 345]. 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-AU

Table 4.5.2.1: Proposed Staff in SRA-AU

	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-AU

	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 in ammonia combustion requires an online analysis of the 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 €).

- Kneer 60k€: Dynamic Phase Transition Evaluation Rig
- Pischinger 75k€: Ir camera and optics equipment
- Pischinger 100k€: Adaptation of optical single-cylinder engine
- Schröder 100k€: Micro PIV system incl. microscope
- Palkovits 100k€: Online Analysis Ammonia Decomposition (MS)
- Mechler 120k€: NH3 fuel cell test station

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 €).

- Pischinger 150k€: Adaptation of cylinder head for thermodynamic investigations
- Boxx 156k€: Optical Parametric Amplifier (to be combined with the femtosecond laser system acquired by WSA through TMFB cluster to build a 2-photon LIF imaging system for ammonia and currently experimentally inaccessible species such as atomic N, O and H) shifted to CBFA?
- Pischinger 165k€: Flex-fuel, reversible DL-SOFC single cell test bench (upgrade of preexisting system): Vaporizer (for electrolysis operation) Power-Source (for electrolysis peration) Externer Reformer Electrochemical impedance spectroscope (EIS)
- Palkovits 250k€: Parallelized gas-phase reactor for Ammonia Decomposition

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 ([76]). 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 22). 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.

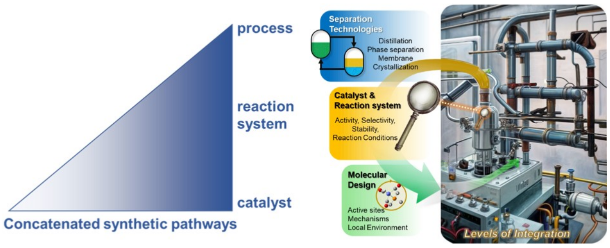

Figure 22: Holistic design of concatenated synthetic pathways considering the various options on the levels of catalyst, reaction system, and reactor and process design for an overall optimum.

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

Klanker-mayer

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.

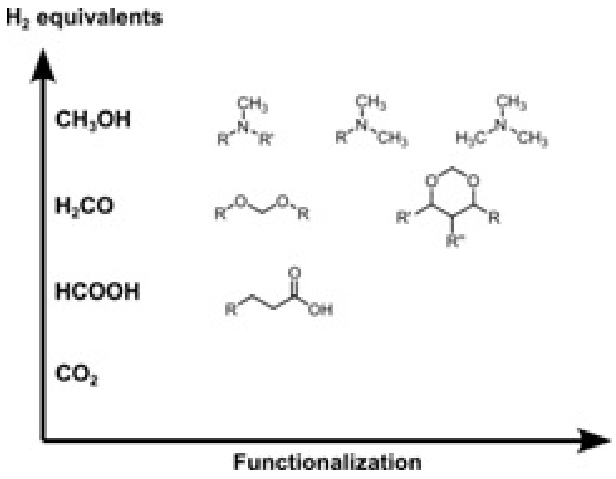

Figure 23: ?

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 [77]. 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 [REF]. This includes new strategies for the reduction of CO_2 to formic acid as well as methanol with molecular REF or solid catalysts [78] providing flexibility with regard to operation in multiphase REF 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 [REF]. 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 [REF].

Utilising ligand structures as building blocks of materials, solid molecular catalysts based on mono- and bidentate phosphines, pyridine and triazine motifs and lately even tert-pyridine structures could be derived. Their use in both continuous liquid as well as gas-phase catalysis was demonstrated. E.g., 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 (REF). In contrast, for polyphosphines superior activity and selectivity of isolated metal species in CO_2 activation to formic acid was confirmed.

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 [REF] to the synthesis of for linear and cyclic acetates as bio-hybrid fuels by valorising various biogenic alcohols [REF] or plastic waste [REF]. The concatenation of bio- and chemo-catalytic steps was successfully demonstrated already for some selected cases by interdisciplinary collaboration of FSC teams. [REF].

Major challenges can also be found in the selective hydrogenation of CO and CO_2 to higher alcohols where methodologies to derive C_{2+} alcohols remain rare [79, 80]. In an innovative approach, Fischer-Tropsch synthesis to olefines was combined with reductive hydroformylation [81] A heterogeneous cobalt catalyst with high olefine selectivity could be integrated in tandem with thermostable cobalt reductive hydroformylation catalysts to realize a slurry-phase direct conversion of syngas to higher alcohols. The first example of a Rh-based catalytic system capable of direct conversion of 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. [82]

Carboxylic acids beyond the simple hydrogenation product formic acid are highly interesting product targets that could be assessed from CO_2 by concatenated reaction principles. 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 [REF]. The 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 [REF]. 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 [REF]. 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 [83]. 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. [84]

Electrocatalytic carbon dioxide reduction (CO2RR) [85] has also significantly evolved in recent years allowing access to e.g. CO, formic acid or ethylene [86]. 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 [87]. 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. [88, 87]

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 [89, 90]. In FSC, the catalytic toolbox could be significantly broadened by utilising electrocatalytic biomass valorisation, e.g., for valorising 5-hydroxymethylfurfural [REF]. Kolbe electrolysis was explored due to its potential to transform biogenic carboxylic acids to monomers and fuels [91], e.g., by electrochemical cross-coupling of biogenic di-acids allowing to flexibly tailor the fuel structures [92]. 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 [93]. 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 ?[**?**]. 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 [70, 94].

The Integrated Fuel & Chemical Science Center (FSC^2) Principal Investigators (PIs) also made first steps into the integration of nitrogen functionalities in the valorisation of renewable feedstocks, e.g., via both chemo- and electrocatalytic amination and amidation of biogenic carboxylic acids. Therein, a 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) highlighted the environmental and economic potential of this route. Indeed, LCA projected that bio-based NVP production reduces global warming impacts by 25–53% compared to the fossil alternative practiced today. [95]

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. [96] On top, by the combination of 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.

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

Aiming at a catalytic toolbox to provide a flexible bio-hybrid platform made of molecular building blocks that can be integrated into resilient material cycles, methodical advance enabling the sustainable formation of C–C, C–H, C–O, and C–N bonds, is sought for (Figure 24). 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- [REF] 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

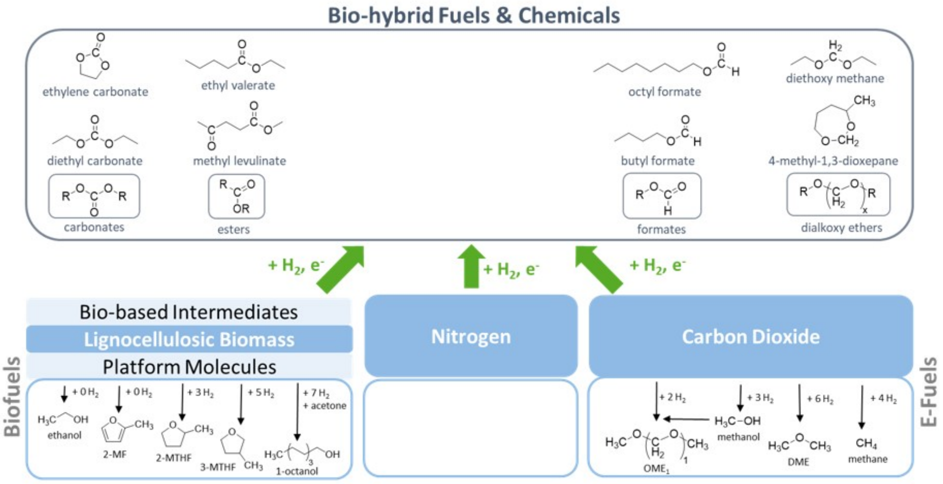

Figure 24: ?

recently for the selective β-methylation of alcohols [REF], the platform will serve as a starting point for new catalytic approaches towards C-C bond formation (N.N.). 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.

As an example, combining synthetic organic chemistry with computational and mechanistic studies, Schoenebeck group uncovered novel catalysis principles based on multinuclear metal catalysis, (i) metalloradical catalysis, (ii) the unlocking of orthogonal reactivity space with organogermanes, and (iii) uncharted chemical space of N-CF3 (and N-CF2H) compoundsiv. Therein, the group showcased how machine learning methods can be used to accelerate identifying catalyst design of previously unknown dinuclear Pd catalysts REF. In FSC^2, this approach will be advanced further and applied to exploit catalysts enabling C-C and C-N bond formation.

Strategic sentences on automation, parallelization, data-driven methods, novel Professorship
More high throughput, ML?

4.5.3.2 Interconnected Catalytic Concepts

Rother

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 [97]. 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 [98]. 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 [99, 100]. 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 [101]. 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 [102]. 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 [28]. 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 [103] and biocatalysis in unconventional media [104] 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} [105]. 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 [106, 107]. 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 [108]. 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 [109]. 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 [110], 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 [111].

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)

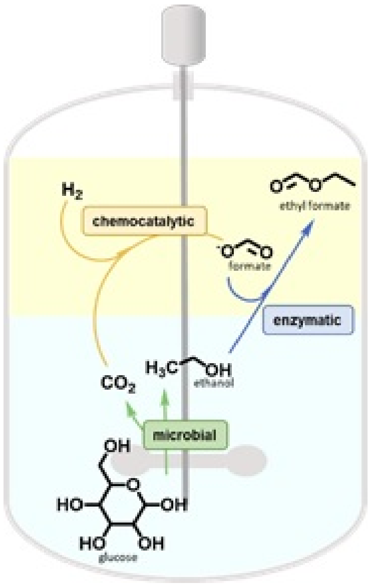

Figure 25: Combination of microbial, chemocatalytic, and enzymatic catalysts for the integrated synthesis of ethyl formate from biomass and CO_2 in a one-pot, two liquid-phase reactor.

4.5.3.3 Integrated Reactor Systems

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 [112]. This reactor as a one-pot reactor combines biochemical conversion with a corresponding separation sequence without simultaneous loss of yield [113]. 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 [84, 114]. With the proposed integrated ISPR concept, the carbon dioxide emission of the microbes can be used again as educt for the chemical conversion [108].

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 [115, 116]. 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 [117, 118]. 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 [37, 119]. 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 26 [120]. 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 [120], but trace metal impurities decrease the selectivity. These can be overcome by a resting cell approach in the fermentation step [121].

Another way to improve electrochemical reactors is by using the dynamic extension of electrochemically active surface area by flow electrodes or slurry electrodes [122, 123].

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 [124] enables, in combination with steering the process conditions, a high degree in control over the reactor's selectivity. [124] In a next step, several tubular electrodes were integrated into one reactor, which enable swift scale-up via numbering-up (Figure 27) [125, 126]. 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 [127, 122, 128, 123].

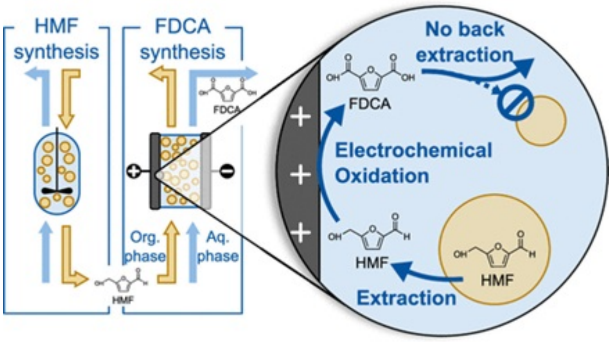

Figure 26: Integrated conversion of fructose to FDCA in a biphasic systems comprising chemical and electrochemical conversion.

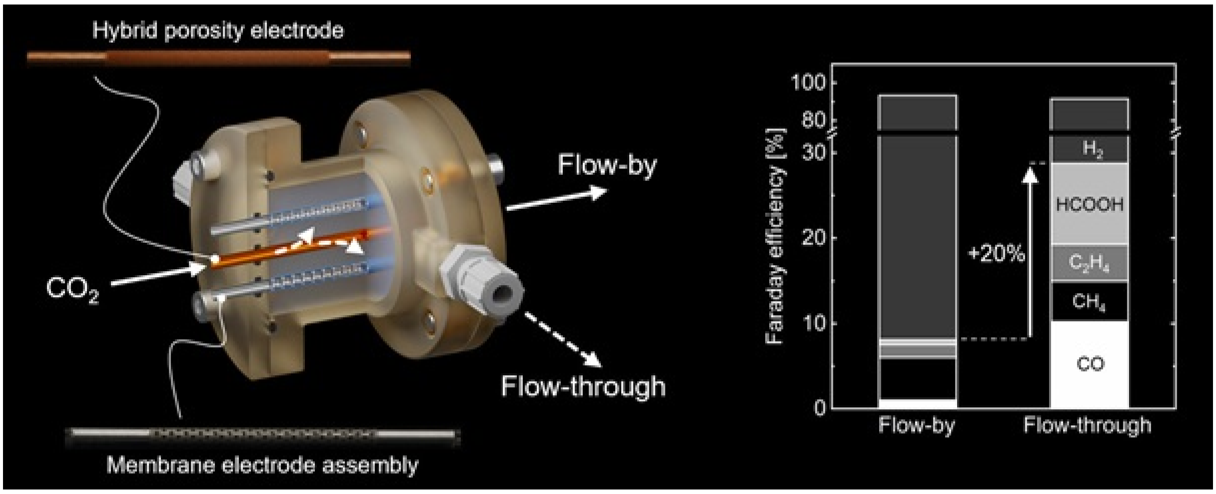

Figure 27: Flow reactor for 3D printed tubular gas diffusion electrode with tailored porosity.

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.

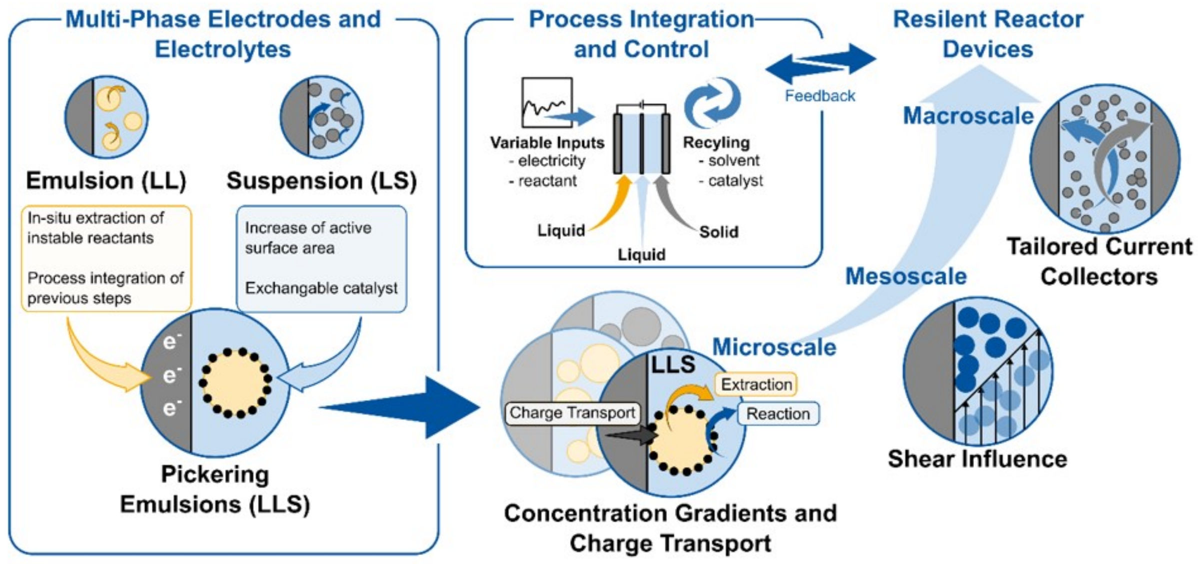

Figure AAA Scale based approach for multi-phase electrochemical systems.

Figure 28: Scale based approach for multi-phase electrochemical systems.

Figure 28 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.

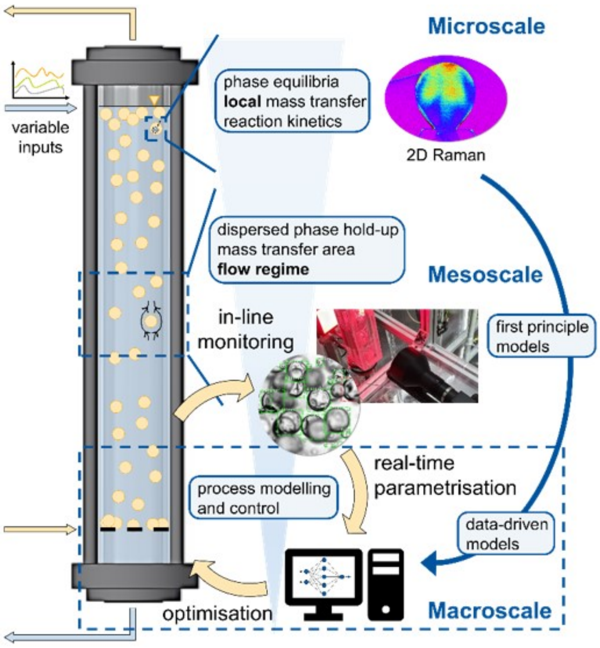

Figure 29: Autonomous and self-optimising multi-phase tubular reactor.

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 €

- Klankermayer 125k€: High-pressure equipment with adapted analytics
- Jupke 120k€: High-pressure Differential Scanning Calorimetry
- Palkovits 120k€: Multi-fold parallel pressure reactor (e.g. Batchington from Avantium)
- Jupke 50k€: High-pressure density meter
- Jupke 60k€: 3-phase tailor-made measuring cell
- Lauterbach 90k€: NMR benchtop spectrometer for in-situ product analysis
- Palkovits 50k€: Online Benchtop NMR for analysis
- Blank 50k€: Automated microbial genome editing workbench
- Blank 50k€: TOM Microbial Physiology Workbench

Instrumentation above 150 000 €

- Blank 18050k€: 2x DASbox Mini Bioreactor System

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 30, left). 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 (Figure 30, right). 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 30: ?

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 ([129]). A specific microbe could be engineered to produce 3-(3-hydroxyalkanoyloxy)alkanoic acid (3-(3-hydroxyalkanoyloxy)alkanoic acids (HAAs), [130]) as platform intermediate for chemo-catalytic or electrocatalytic [131] 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 [132].

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 [133]. 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 [134]. For example, 2,3 butanediol was recovered by this technology from microbial fermentation broth [99]. 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 ([135, 136, 137, 138]).

Recently, we could showcase that CO_2-derived substrates such as formate and acetate can be metabolized by smut fungi, [84] 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 [114, 139]. In the FSC, the synthesis of formate and acetate from CO_2 was studied extensively [140, 141, 142, 143]. 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 ([108], Figure 31).

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

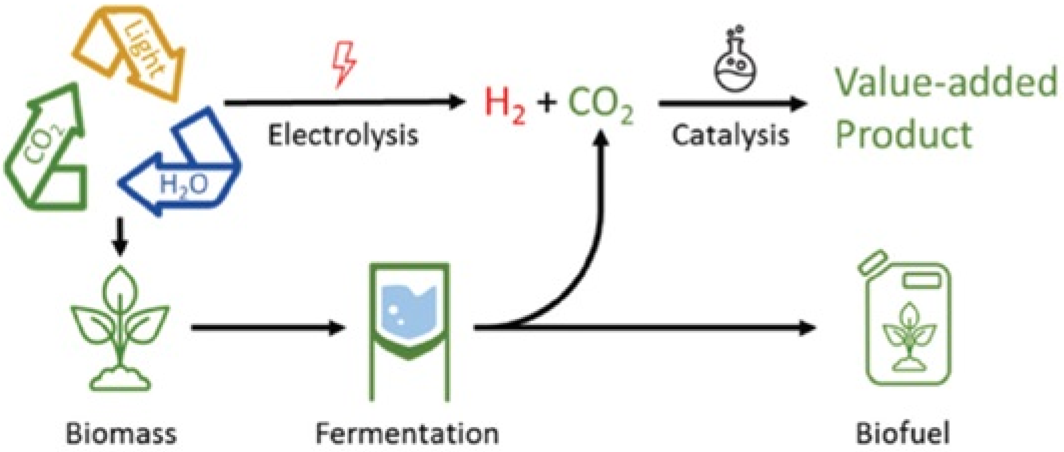

Figure 31: Utilization of renewable resources for biofuel production through fermentation and additional catalytic CO2-reduction to value-added products. [108]

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 using a borescope under operando conditions using a specifically designed high pressure reactor was crucial for the understanding of the complex phase behaviour ([144, 145]).

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 [146]. This provides access to another important source of carbon within the systems boundaries of a de-fossilized value chain [147, 148].

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 [149]. 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 [150] 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.

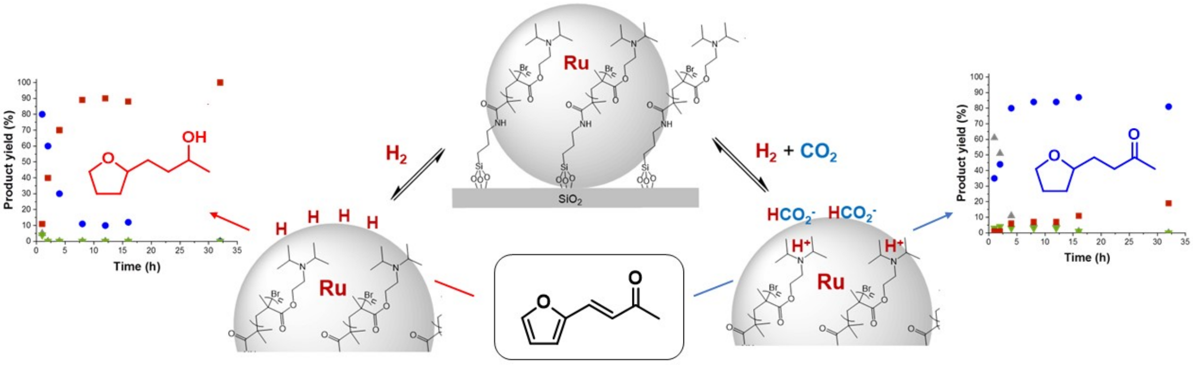

Figure 32:* *Adaptive catalysis produces either the fully saturated alcohol or the partially saturated ketone from bio-based furfuralacteone depending on the use of pure H_2 or H_2 in presence of CO_2. [149]

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 [151, 152]. 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 [121]. 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 [153]. The newly acquired experience of the Waldvogel team with scalable electrosynthetic methods utilizing technical grade feedstocks will be highly beneficial in this context [154].

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 [155] 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 [156, 157, 158].

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 [159] beyond simply replacing thermal with electrical heating. 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[160]. The potential of solid-state NMR to obtain fundamental insights into mechanochemical processes has been demonstrated and critically discussed[161]. 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[161]. (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 [93]. 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[121].

?[162]

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 [163]. 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

[164].

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
[161]

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).[**?**, 165][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 [166]. Both, combined temperature and vacuum swings as well as sorption and regeneration cycles without vacuum swings confirmed high stability of the best performing materials (Figure 33).

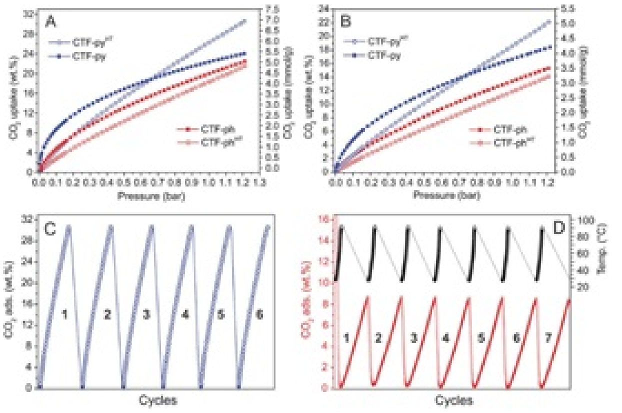

Figure 33: Check: Low-pressure CO_2 isotherms of CTF-ph ( ), CTF-phHT ( ), CTF-py ( ), and CTF-pyHT ( ) measured at A) T = 273 K and B) T = 298 K. C) Six cycles of CO_2 uptake at T = 273 K on the CTF-pyHT sample. D) Seven cycles of CO_2 uptake at ambient temperature and pressure for CTF-pyHT . TGA measurements (red curve) refer to the CO_2 uptake/release throughout the temperature heating/cooling cycles (black curve). [166]

Also, polyacrylonitrile-based carbon nanofibers (CNFs) were prepared at different carbonization temperatures, and the resulting fibers were analyzed with respect to CO_2 sorption using dynamic sorption techniques [167, 168]. The best performance was found for the CNFs prepared at 600°C with measured CO_2/N_2 selectivity values of up to 194. Again, a medium temperature of the material pretreatment proves to be advantageous, corresponding to the trade-off between material hydrophobicity and N-content [168].

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 [169]. Also, along the value chain of high temperature co-electrolysis of CO_2 and

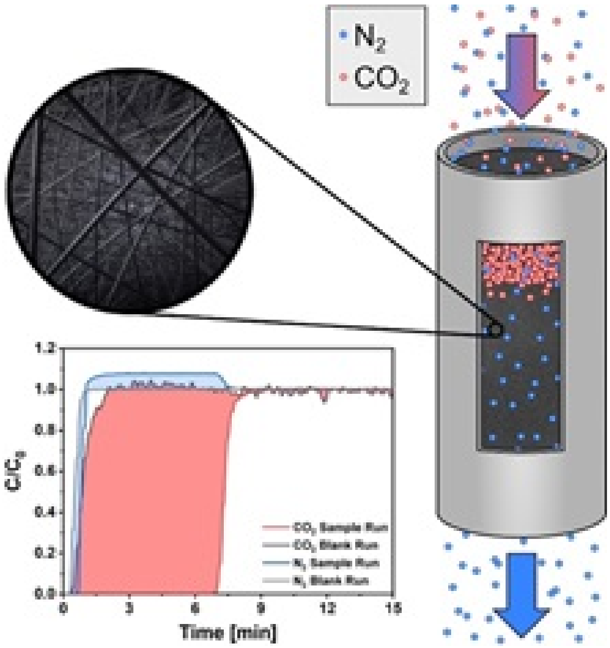

Figure 34: Breakthrough curves. Adsorption was performed with 50 % He, 45 % N_2, and 5 % CO_2 at 273 K and 5 bar on PAN-based CNFs carbonized at 700°C and is shown in comparison to a blank run. [168]

water to CO and H_2 followed by CO_2 hydrogenation, direct integration could be demonstrated [170]. 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. Further studies on impurities effects of CO_2 feeds showed a positive effect of trace amounts of oxygen enhancing catalytic activity for CO_2 methanation e.g. more than doubling the reaction rate at 300°C [171]. The effect is still not fully understood, though, surface hydroxylation potentially facilitating substrate adsorption appears to play a role.

- Previous work Leitner, Jupke[115, 172, 116], Blank[108], Palkovits[169]

On reactor and process level, previous studies also investigated up- and downstream integration, CO_2 conversion and electrochemical pH management. First examples highlight that integrated carbon capture and conversion brings about several advantages with respect to substrate utilization and energy efficiency.
Indeed, productivity and selectivity of the thermo-catalytic hydrogenation (Ruthenium-based catalyst) of CO_2 to produce carboxylic acids (e.g., formic acid) could be significantly enhanced by supplementing the primary liquid homogenous reaction phase (decane) by a second liquid product conservation phase (methanol) wherein the product was continuously extracted by an acid-amine complex [1,2]. In [3], a two-phase system was applied to utilize the co-produced CO_2 of a bioethanol fermentation as a feedstock for a homogeneously catalyzed hydrogenation (Ruthenium complex) to produce formic acid. To avoid the use of acid and base for pH

control in aqueous systems and significantly reduce the co-produced saline waste, we developed electrochemical pH shift cells directly producing H^+ and OH^- ions for pH control [4]. We applied this technique to develop in situ purification processes particularly for microbially produced carboxylic acids [4,5,6].
not used text

- Wessling group on CO_2 capture [173, 174, 175]

Beyond CO_2, also the selective separation of biomass-based intermediates such as sugars, carboxylic acids, amino acids and diols[176, 177] 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

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 (Wessling). For high Faraday efficiencies and carbon utilization, pH 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 establish the required protons, which shift the equilibrium for bicarbonate to dissolved CO_2. With precisely designed porous 3D electrodes we aim to control mass transfer and pH gradients inside the electrode and thus ensure sufficient reactant availability while preventing oversaturation of the electrolyte and subsequent CO_2 bubble formation. Multiphase modeling (Pitsch) will accompany dedicated experiments to elucidate bubble nucleation, detachment and removal in complex electrolytes and electrode structures.

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 temperature) and converting (high temperature) 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 valorizing sorption enhanced catalysis (Palkovits). Conceptually, sorption sites close to the active centers cause locally enhanced substrate concentrations directly translating into superior reaction rates far beyond the limitations of the bulk feed concentration. Understanding necessary molecular proximity.

SEE ALSO:

On the system level, the methodological concepts are mirrored in dynamic modelling of material behavior and LCA for Designing Sustainable Integrated Carbon Capture and Conversion Processes in Volatile Energy Systems (van der Aßen). The role of Combining Single reactor avoids CO_2 transport and enables heat integration between the CO_2 capture and conversion steps.

4.5.4.4 Proposed Staff and Funding of SRA-TCP

Table 4.5.4.1: Proposed Staff in SRA-TCP

	2026	2027	2028	2029	2030	2031	2032
Staff category	**Number of persons**						

Continued on next page

(Continued)

	2026	2027	2028	2029	2030	2031	2032
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	16.5	16.5	16.5	16.5	16.5	16.5	16.5
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)	1257	1295	1334	1374	1415	1457	1501
Direct project costs (excluding staff)	240	370	195	195	195	195	195
Total instrumentation < €150,000	475	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 €

- Wiegand 100k€: HXY triple-resonance solid-state NMR probe (500 MHz), also capable for low-gamma nuclei
- Kneer 100k€: Microscopic fiber-based cavity-enhanced spectroscopy system (anderes SRA??)
- Zobel 120k€: CHNO analysis
- Leitner 130k€: Bruker IR 70V
- Jupke 60k€: Multi-phase reactor
- Mechler 85k€: Experimental setup to operate at elevated current densities and potentials: Bipotentiostat with boosters, cells and pumps
- Simon 70k€: MW-cavity for X-Ray spectroscopy and diffraction

Instrumentation above 150 000 €

- Magnus 160k€: Dasbox (das gleiche wie Blank?)
- Jupke 150k€: Online analytics suited for high temperature reaction systems (e.g. NMR, GC)

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 Life Cycle 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 developed process paths, chemicals, and fuels must then be integrated in 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, the life-cycle assessment methodology is extended to capture the environmental impacts of fuels and chemical conversion systems over all scales. Ultimately, life-cycle assessment is 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.

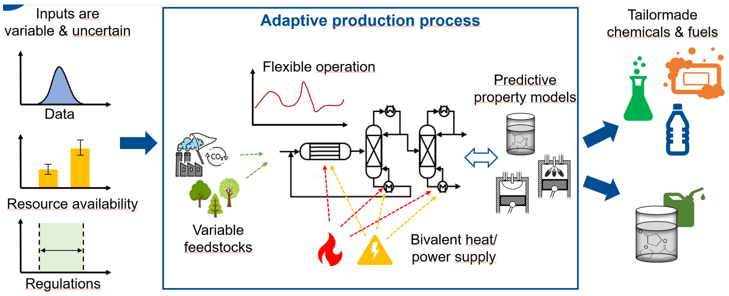

Figure 35: Rough draft of fuel design for resilience and adaptivity

4.5.5.1 Fuel & Chemical Design

Mitsos

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 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 ..., 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.

Walther

4.5.5.2 System integration

The aim is to design resilient, adaptive, and sustainable conversion systems for fuels and chemicals using an integrated approach based on system analyses, 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 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 analysed conditions for market adoption and diffusion of bio-hybrid fuel value chains. Combined micro- and macro-level analyses ([178]) 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 ([179, 180, 181]AmiriZenodo24). (Meta-)analyses provided predicted future demand of fuels for different scenarios ([182]). Prospective fuel candidates were determined regarding market diffusion barriers and sustainability factors with a possibility-based multi-criteria approach ([178, 183]Hendiani24). *In FSC^2, such analyses gain even more importance with the current discussion on the role of chemical energy carriers, storage options, fuels as well as potential platform chemicals.*

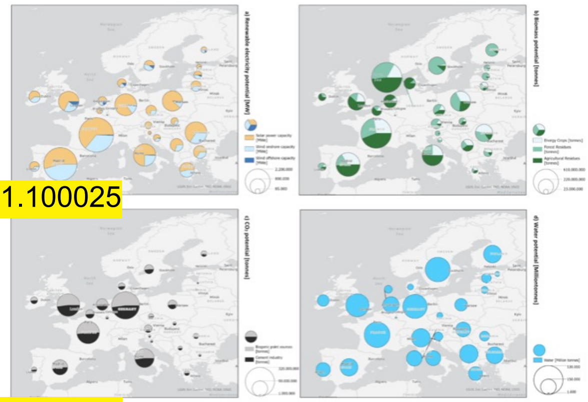

Figure 36: Potential of resources in EU countries a)Renewable electricity potential b)Biomass potential c)CO2 potential d)Water potential [180]

Public perception was analysed FSC as multi-faceted perspective of risks and benefits of fuel products, production processes and infrastructural changes doi.org/10.1016/j .enpo l.2018.10.039 / doi.org/10.1016/j .apenergy.2019.04.041 / doi.org/10.1016/j .egycc.2021.100025 / doi.org/10.1016/j .enpo l.2020.112071 / doi.org/10.3389/fenrg.2022.989553 based on a multi-stage iterative empirical methodology doi.org/10.1016/j .enpo l.2020.111586 / doi.org/10.1186/s13705-023-00412-5 / doi.org/10.1016/j .erss.2018.09.017 . 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 [184] and individual factors [185]. A positive perception of alternative fuels doi.org/10.1016/j .eist.2019.05.003 / doi.org/10.1016/j .egycc.2021.100025 requires comfort and affordability as well as environmental and toxicity benefits of fuels along with infrastructural developments and political communication doi.org/10.3389/fenrg.2022.989553 / doi.org/10.3389/fenrg.2020.579814 / doi.org/10.1016/j .rser.2021.110873 / doi.org/10.3389/fenrg.2018.00073 / doi.org/10.1016/j .eist.2019.05.003 . 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 [186, 187, 188, 189, 190]. *Further extending these results, research in FSC^2 has to overcome segmented and isolated technology-related risks by a systemic risk approach, and an integrated risk communication framework must be developed to support informed decisions and align public and expert views [191].*

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 [183](Torkayesh1d, Torkayesh1e,). Also, the techno-economic

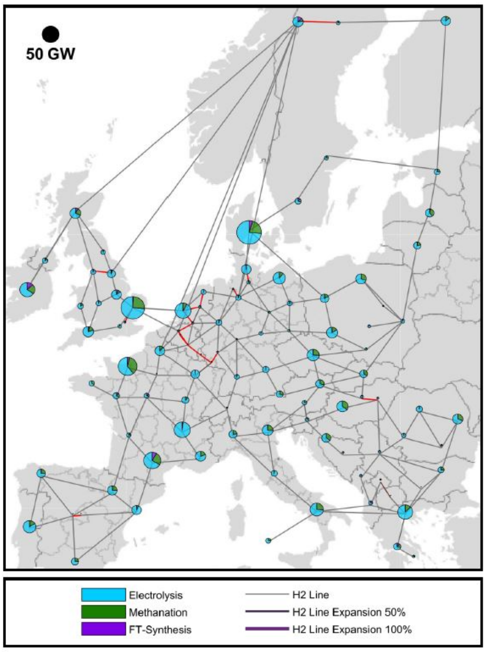

Figure 37: Potential Distribution of Power-2-X Plants in 2050 [193]

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 [192]. *In FSC^2, 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.*

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 [194, 195, 181, 196]. Myopic solution approaches proved appropriate as they reducing the computation time drastically while still providing adequate objective values [181]. On the other hand, value chain models 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 [179]. 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 [193]. Model extensions explored the trade-offs between cost, land-use, and water-use [180], the consideration of policy requirements [197, 198]Zardoshti;, and the innovative integrating of social acceptance in the optimization-based design of bio-hybrid fuel supply chains via multi-objective optimization [199, 200]. 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 [201]. *An extension towards fuel and chemical conversion systems in FSC^2 will be even more demanding and requires more advanced models with extended system boundaries and more flexibility in process paths and fuel types, and specific emphasis on the the system's interlinkages, uncertainties and resilience.*

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.
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 (*Mitsos, van der Aßen, Walther, Venghaus*) and active exchange with the other SRAs of FSC^2 to integrate data and results. Challenges result from the broad system boundary and integrating the hierarchy's device – process (path) – supply chain in sufficient accuracy. This cross-sectorial, hierarchical model lays the foundation for the integration of measures against uncertainties and systemic risks, stakeholder perspectives and policy design

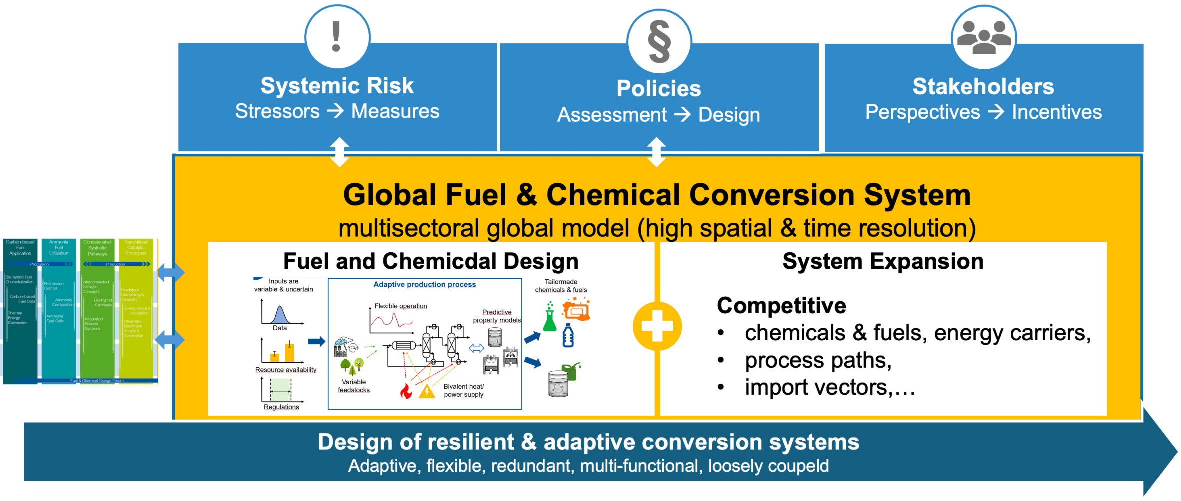

Figure 38: Design of resilient and adaptive conversion systems by integration of stakeholders' incentives, policy design, and systemic risk measures

(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., [202]). FSC^2 replaces the so far often 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 [203, 204, 205, 206]Arning/Venghaus. Thus, we overcome the centralized perspective that omits stakeholder-specific decisions (e.g., [207, 208, 209], 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. Integrating these results into the prescriptive model for resilient fuel value chain design allows to regard for interrelations and synergies between policy design and resilient system design.

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.

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4.5.5.3 Life-cycle assessment

To enable the The Fuel Science Center (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 impacts and process interactions holistically, reliably and on a broader scope. 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 in LCA to improve the reliability and resilience of sustainable fuels.

The methodological research will be accompanied by the application of investigated chemical conversion systems, e.g. ammonia synthesis, integrated 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 environmental 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 [19].

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 [346, 347].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 [348].Furthermore, as we continue to expect to obtain fuel blends (such as KEAA) in FSC^2, the assessment of mixture toxicity is important. Previous work in FSC has shown that ... [Karsten Braun’s work, FSC presentation and award, however no publication found?!] In addition to experimental toxicity assessment within FSC, Backhaus et al. have assessed approaches for toxicity prediction for mixtures [349].LCA has been applied to chemical conversion systems on a molecular and process scale to guide catalyst design and electrochemical synthesis [253, 254].As core concept of FSC, the fuel design aims at identifying

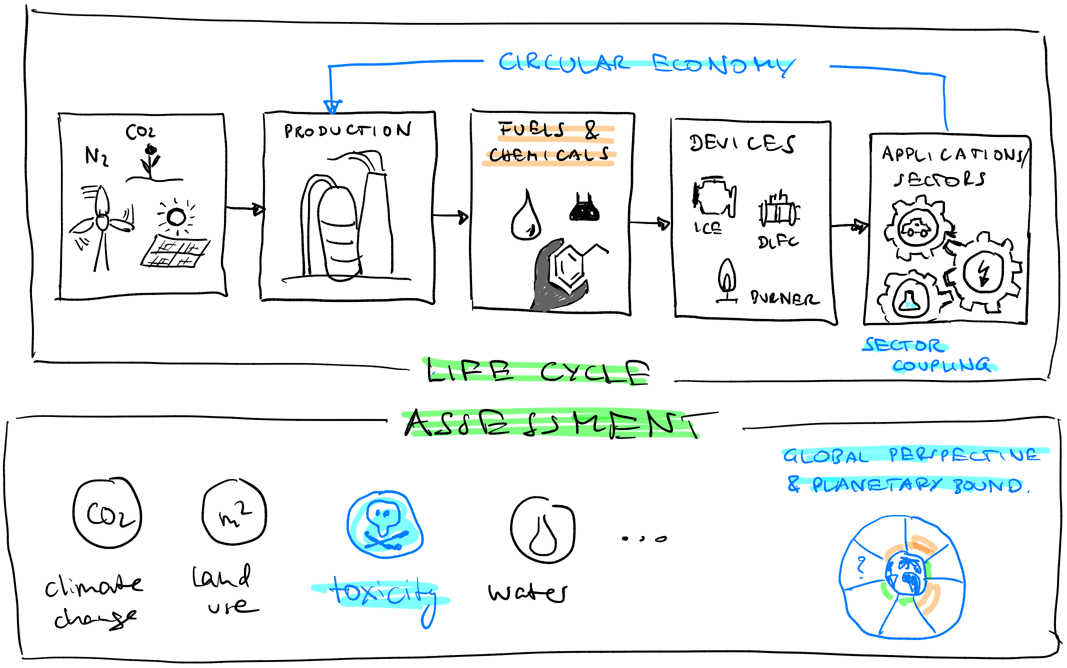

Figure 39: LCA will be applied to the production and conversion of fuels & chemicals. LCA will be extended methodologically (extensions highlighted in blue): toxicity prediction, sector-coupling, planetary boundaries and circular economy.Figure needs to be 'professionalized'

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 [**?**].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) [255] and to evaluate whether and how DSM offers environmental benefit [256, 257]. 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 [258].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 [259, 260] and systematically reviewed product quality aspects for waste recycling within LCA [261].

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 [210]. 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 [262] , 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 environmental 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 LCA methodology to account for anthropogenic stock changes and product quality

Work program

The common approach in this sub-SRA is to apply and advance the methodology of LCA 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 LCA assessment results as output to steer further technological research. For example, LCA will be used to identify the environmentally and technically most promising application areas of direct liquid fuel cells (DLFCs) (see XY.). During application of LCA, we will conduct research on the LCA methodology itself for its further advancement. The description of the work program will focus in the methodological LCA 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, 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. mention platform for data exchange? Research Data Management 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. 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.

- describe benefits of sector-coupling and motivate scope extensions - describe models (SecMOD, energy system, existing sectors and products) and methods, incl. transition pathways

Similarly, 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	0	0	0	0	0	0	0
Postdoctoral researchers	0	0	0	0	0	0	0
Doctoral researchers	15	15	15	15	15	15	15
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

Guidelines for section 4.6:
If applicable, please provide information regarding important legal and/or ethical topics in research. please provide a concise but sufficiently comprehensive explanation in keeping with the relevance of each topic to the proposed research. If any of the following topics are of central importance to the research questions addressed by any subunit of the research programme, discuss them in the respective part(s) of section 4.5 and reference them accordingly in the following section:

- General ethical aspects
- Descriptions of proposed investigations on humans, human materials or identifiable data
- Descriptions of proposed investigations involving experiments on animals
- Descriptions of projects involving genetic resources (or associated traditional knowledge) from a foreign country
- Explanations regarding any possible safety-related aspects (“Dual Use/Research of Concern; foreign trade law)

For detailed information on these topics and the formal and legal requirements, please refer to the instructions for proposal preparation and submission and the references they contain:
`https://www.dfg.de/formulare/exstra131`

Estimation: In total, a maximum of 1 page for this section.

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

TMFB/FSC publications

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Guidelines for section 5.1:
Explain what strategies and measures will be implemented by the Cluster of Excellence to support early-career researchers at their respective levels of qualification. If applicable, describe their integration in existing or planned early-career support structures, such as graduate schools, etc. Refer to the current situation regarding early-career researchers and existing strategies for early-career support and staff development at the applicant university/universities and within the participating departments and/or faculties. What aims have the participating departments and/or faculties set themselves in this area? How do the objectives and activities of the Cluster of Excellence fit into or complement these?
Renewal proposals only: Please describe the relevant achievements of the first funding period.
Please summarise the requested funds for these measures using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table, and that "Instrumentation" refers to all instruments, software and other equipment costing more than 50,000 euros per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 3 pages for this section.

5 Structures and strategies in the Cluster of Excellence

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

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							
Direct project costs (excluding staff)							
Instrumentation							

Guidelines for section 5.2:

Please describe the aims of the Cluster of Excellence with regard to supporting equity and diversity. Explain what measures will be taken to achieve these goals, with reference to the DFG's Research-Oriented Equity and Diversity Standards:

`https://www.dfg.de/equity_diversity_standards`

Refer to the present situation at the applicant university/universities and within the participating departments and/or faculties, and – in the case of renewal proposals – within the Cluster of Excellence. What objectives have the participating departments set themselves (qualitative objectives and additionally – for male and female researchers only – quantified targets)? How will the Cluster's activities be incorporated in the relevant equity and diversity strategies at the university/department/faculty levels? please highlight particular efforts relating to gender equality.

Renewal proposals only: Please describe the relevant achievements of the first funding period.

Please summarise the requested funds for these measures using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table. "Instrumentation" refers to all instruments, software and other equipment costing more than 50,000 euros per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 3 pages for this section.

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

Carmen Leicht-Scholten - Project proposal:
Extensive literature research and analyses were carried out from a perspective of gender-sensitive science and technology studies that acknowledge given interdependencies between scientific, technological, and societal development (Leicht-Scholten 2007; Leicht-Scholten 2018; Ernst and Horwath 2014; Bauer, Voigt, and Lemke 2017). Thereby, we 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, we researched the general relationship between gender and sustainability while considering intersectional factors and how to connect these insights to engineering processes (Bosen et al. 2023). The findings of this research highlight that 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 (Khalikova 2021; Odrowaz-Coates 2021; Prati, Cazcarro, and Hazra 2022). 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. This is because petro-masculinity highlights the fact that fossil fuels contribute to more than energy consumption and related profits (Daggett 2018). They further contribute to the formation of identities that construct masculinity and femininity oppositely and in a state of inequality, which perpetuates existing injustices (Daggett 2018). 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 (Hedenqvist et al. 2021; Stoddard et al. 2021; Hultman 2021; Pulé and Hultman 2021; Daggett 2018). 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). Taken together, this conceptual basis builds a transformative lens for the research done in the cluster that critically informs researchers about social, economic (political), and environmental factors of the design, implementation, and use of their research, which, ultimately, fosters social justice and sustainable development (Mertens 2021). Further, this fosters inclusivity and participation within the cluster and, additionally, motivates for ethical usage of research findings towards societal ends (Mertens 2021).

Adopting this perspective makes it possible to contribute to the sustainable development of fuels on the one hand, and on the other to establish 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 our system-theoretical approach to diversity management (Steuer-Dankert and Leicht-Scholten 2022; Steuer-Dankert and Leicht-Scholten 2019; Steuer et al. 2017), we assessed the organizational diversity of the cluster based on the factors of gender, internationality, and position. While this offered first insights into the diversity and reality of the cluster, we wanted to broaden this perspective for structural and scientific purposes. Accordingly, we developed – together with the Office for Data Protection at RWTH Aachen – a novel study design that follows the theoretical framework on diversity in terms of Gardenswarts and Rowe's (2008) that conceptualizes diversity into internal, external, and organizational dimensions with personality at the center of diversity. The study allows us to gain insights on the following dimensions of diversity while being voluntary and completely anonymous and non-traceable: 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.

Taken together with the established theoretical background, this picture of the diversity of the cluster can then serve as the basis for an initial needs-orientated workshop that brings these topics together with the reality of the cluster and its employees. Prof. Martin Hultman from Chalmers University, a renowned international researcher in the field of gender-sensitive science and technology, whose research focuses on petro-masculinity and sustainable development, has already been recruited for this first keynote and workshop. Furthermore, a prototype of a study design was developed, which allows to research and evaluate the effect of the event. 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.

In addition, we further sketched our future work within the cluster and established a plan for a series of workshops that can follow up on the first workshop; see below.

Specific (innovative!) research objectives:

- Workshop on Experiences of Discrimination within Scientific Research Organizations
- Workshop on Inclusive Communication within Scientific Research Organizations
- Workshop on Guidelines for Communication and Collaboration
- Pre- and post-studies around the workshops to explore the level of knowledge and attitudes towards the topic of gender and diversity among the cluster members
- Knowledge transfer in the research community of the cluster as well as in gender studies or even the industry

Research hypotheses and/or questions:

- How can gender studies contribute to the sustainable development of transformative fuels?
- How can gender studies contribute to the establishment of an inclusive scientific research organization?

Research methodology:

- Hermeneutics
- Literature Reviews
- Quantitative Studies
- Qualitative Studies (optional)

Contribution to the overall objectives of the cluster:

- As the inclusion of gender and diversity fosters innovation, our project contributes to all objectives by supporting the development of an open, inclusive, and thriving research culture that is open to novel ideas. Further, inclusive cultures and organizations attract diversity and excellence in terms of personnel development, which, of course, further contributes to all objective and scientific excellence in general.

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							
Direct project costs (excluding staff)							
Instrumentation							

Gleichstellung & Diversität
Gender Equality
Equality between men and women is a key focal activity within RWTH's human resource development. FSC will build upon the university's gender equality initiatives covering a wide range of activities through the RWTH Center for Young Academics:

- Transparent and quality-based selection and recruitment processes monitored by the steering committee responsible.
- Provision of specialized support centers and mentoring programs for female researchers helping them advance their personal and professional competencies and academic key qualifications.
- Dedicated financial support programs to specifically promote the careers of female scientists, e.g, by offering re-entry positions for scientists after parental leave.
- Family support, daycare facilities, and short-term childcare services.

These activities are framed in the "Gender Equality Action Plan (2017 2022) addressing six different fields of action: Cultural Change; Gender Governance; Gender Monitoring; the University as a Workplace; Equal Opportunities and Protection against Discrimination; Research & Teaching.

Whith female scientists represented in leading academic position with only 8 % back in 2008, RWTH has set its general target to a 20 % share of female professors at all levels by 2020. The progress is tracked and monitored annually. By the end of 2016, RWTH already reached a share of 16.5 % of female professors. FSC strives for the overall target of 30 % female scientist among all disciplines and hierarchies, especially through corresponding recruitment activities. With its many new tenure track positions, FSC will thus be pro-actively underpin the ambitious gender goals of RWTH. The University will support FSC during the recruiting process substantially by talent scouting and family-friendly recruiting.

Diversity

RWTH aims to create a flexible and inclusive work or study environment and to realize comprehensive equal opportunities in research and teaching. To meet the increasing challenges and support the potential of diversity, the university has developed a specific diversity policy aiming at opening the university, initiating a cultural change, constructing a life-phase-oriented staff policy, and strengthening of gender and diversity competences. The staff policy and all derived diversity activities are coordinated and reflected on by the so-called “forumDIVERSITY”, a university-wide steering committee.

Since 2013, RWTH’s “Diversity Action Plan has been focusing on the different dimensions of diversity: gender equality, internationalization, family-friendliness, accessibility and inclusion, and educational equality (e.g, support for first generation students and Ph.D.s from non-academic families). FSC intends to recruit 30 % of its Ph.D. student cohort internationally through advertising the positions worldwide. Ethnic diversity for the tenure track positions will receive particular attention while scientific quality remains the leading recruitment criteria.

To create early intercultural awareness already at the Ph.D. student level, training on the matter of “unconscious bias will be compulsory in the FSC Research School.

Family-Friendliness

RWTH offers various measures in place to secure equal opportunities and activities to achieve permanent establishment of a family-friendly work environment such as:

- Support offers for surrounding topics such as starting a family, maternal protection, parental leave, childcare, and the care of relatives (Family Service Center).
- Workplace flexibility e.g., home-office, and situational mobile work.
- Activities regarding a family-friendly leadership, e.g., the brochure “Golden Rules of Family-Friendly Leadership”.

A number of agreements and guidelines provide a framework that supports students and employees in balancing academic and family responsibilities. RWTH has been certified as a family-friendly university in 2009 and was successfully re-auditioned in 2012 and 2015.

FSC will be instrumental to reach the ambitious goals specified in the RWTH Policy. At this stage, FSC comprises 20 % of female PIs in the core team, and two females out of six coordinators of the CAs in the steering committee. In close cooperation with the participating Faculties and the RWTH Integration Team, FSC will coordinate particularly the recruitment of the future appointments listed in Table 5.2.2 to actively search for female candidates.

In summary, FSC will implement the following specific measures to foster gender equality, diversity, and family friendliness:

- a steering committee member responsible for the management of Equal Opportunity and diversity processes,
- individual and partnership coaching and mentoring by the Center of Professional Leadership,
- mandatory unconscious bias trainings from the Ph.D. student level on with increasing intensity during academic development to initiate and sustain continuous awareness building,
- conscious scouting of female postdoc candidates and junior research group leaders to counteract the “leaky pipeline challenge,
- a family-friendly research environment where the FSC Research School encourages in particular male Ph.D. students to take parental leave,
- closely collaborating with the “RWTH Equal Opportunity Office to establish flexible and easy access Child Care Opportunities,
- supporting a culture and flexible digital infrastructure allowing communication and team interactivity combined with flexible home office times (Mattermost hosted at RWTH, cluster-internal cooperation platform),
- lab technician support for pregnant Ph.D. candidates and Postdocs who cannot access labs.

Equal Opportunity Coordination and Funding Requested for Equal Opportunity

The measures for equal opportunity will be centrally coordinated (0.5 FTE, E13) in the Cluster Office. The CoE will fund 0.25 FTE for childcare (S7) for after office hours of public child-care facilities. RWTH will provide the required space close to its core facilities. In addition, the cluster will furnish several parent-and-child offices at its core facilities. Home office will be supported by FSC through supply of required hard- and software in order to keep the quality of communication within the FSC-team as high as possible.

PE & Talentmanagement

Early Career Support at RWTH Aachen University

Early career researchers are the backbone of the research culture and research achievements at RWTH Aachen University and FSC. Investing in the development of early career researchers and their research competences is key to (i) a swift and sustainable development of new research fields as well as (ii) its translation forward to stakeholders and partners outside of RWTH.

Support will be provided for both academic and scientific development. Their academic development progresses under the umbrella of the RWTH Center for Young Academics (see Figure 43) ensuring a university-wide consistent education of all early career researchers. Their scientific development progresses within the Research Schools of the CoEs as described in more detail in the next section. CoE Research Schools will be managed through the cluster's governance.

The RWTH Center for Young Academics with its Research Schools is a vigorous and inspiring learning environment for talent development having diverse backgrounds. The Center for Doctoral Studies (CDS) and the Center for Professional Leadership (CPL) under the roof of the RWTH Center for Young Academics support early career researchers in pursuing their individual career paths either in academia or in industry and society. Measures are getting more individual from career step to career step and will become more topic-specific by integration with the Research Schools. CDS currently offers 57 different courses for the development of general professional and scientific skills and competences. Mandatory courses for FSC Ph.D. candidates and Postdocs address responsible research, scientific integrity, research data management, interdisciplinarity and teaching skills. The CPL offers workshops and individual peer group and team coaching to prepare talents beyond the Postdoc period for different career paths in science and research development through (i) about 20 different courses for tenure track candidates, (ii) a 100-day onboarding for new faculty members, about 50 courses for Postdocs and Junior Research Group leaders, and (iv) an Advanced Talents Program under the patronage of the Vice Rector for "Gender and Diversity". The Advanced Talents Program prepares early career researchers for applications in highly competitive personal grant programs such as DFG Emmy Noether, EU Marie-Curie, ERC Starting Grants.

Early Career Support at the Fuel Science Center Research School (Jenny Roseboom center for young academics)

The proposed Cluster of Excellence "Fuel Science Center will establish an associated Research School, operated under the responsibility of the FSC Steering Committee. The Research School will offer early career scientists from late-bachelor level to junior research group a unique support environment where they excel and evolve into so-called T-shaped talents: they comprehend systemic complexity (breadth) of a society in an energy transition phase and they specialize in contemporary and future scientific methodologies (depth).

Already from the B.Sc. level on, research-oriented teaching governs the curricula at RWTH with teaching and performing research being inseparable. The FSC Research School manages the interaction between classical university classes and hands-on exposure in FSC-labs on FSC-relevant research questions. While early career development is often considered to start at Ph.D. level, FSC will offer students to start as early as the B.Sc. program. These students can be internal RWTH students as well as those coming from outside through the many exchange programs (see Section 5.3). Individualized cluster-specific mentoring can hence start with the B.Sc. thesis already. The many early career support tools at hand and those to be developed are visualized in Figure 44. Monitoring the progress in skill development of the FSC early career researchers will be the responsibility of the Research School and the supervising advisors. From the early beginning on, supervisors and early career researchers agree upon a mentoring plan.

The FSC early career development system is flexible and tailored to the need of the cluster and the need of the early career researcher. The individualization with respect to content as well as monitoring will be organized through the Cluster Office in cooperation with the academic supervisor. For the Ph.D. students, the program is mandatory. The system is permeable for researchers to join or leave this portfolio according to own interests and ambitions. The program will comprise, e.g., lecture series, weekly seminars, colloquia with external guests (FSC Seminar), rotational lab courses, regular retreats, seasonal schools and young researcher conferences (see chapter 5.3). The FSC Research School will particularly support peer learning, exchange, and networking between their members. For FSC's scientific success, international exchange will be essential. 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 offered through the FSC Research School 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.

Measures of Early Career Development at the Different Stages

Students (B.Sc./M.Sc.): Already undergraduate students have ample opportunities to join the cluster's research domains during their academic incubation phase. In fact, this very early engagement in relevant research activities represents one of the Clusters most unique educational features. Most prominent will be a new international M.Sc. program on Molecular Science and Engineering (MSE) positioned at the interface between Chemistry and Process Engineering with a focus on Sustainable Chemical and Materials Products and Processes. Other cluster-dedicated involvement occurs through different means such as B.Sc. and M.Sc. theses, individual practical projects (Chemistry Department), team assignments (chemical and combustion engineering) as well research assistant bursaries for the CA- and TRT-related projects (10 hours a week). Through the network of the FSC, and in particular through the IAB, B.Sc. and M.Sc. students have easy access to FSC-related industrial and international internships. This first exposure to the multi-disciplinary nature of the cluster's research forms the basis of a unique educational profile. Close interaction between research groups and students allows the identification and support of high potential early career researchers. The consistent and continuous scientific mentoring will ensure the adjustment between master thesis and the research concept for the following doctoral phase. Adopted from the DFG Graduate School AICES at RWTH Aachen, individualized master programs serve as an add-on to the regular curriculum within an Honors Class Framework. Like the Dean's List of the Faculties, this early FSC-integration is a measure to identify exceptional talents and expedite their development. It will allow excellent students to shorten the time from bachelor graduation to a doctoral degree down to five years and below. Doctoral Researchers: Potential candidates will be attracted from inside and outside RWTH through open advertisements. FSC's ambition is to attract at least one third external candidates in order to stimulate creative diversity. FSC's target group are the top 20 % of the Masters students based on their written application, grades, and duration of studies. The interview procedure is led by the PI and coordinated through the Cluster Office. Together with a letter of recommendation, a presentation and interviews among FSC PIs, the candidates enter the program of the FSC Research School. A mentoring agreement is signed mutually between the Ph.D. candidate and the supervisor specifying the rights and obligations of both. Developing within the FSC Research School program enables the Ph.D. candidates to perform autonomous research. To guide doctoral researchers through the dissertation project, they will be offered a portfolio of educational, advisory, and service measures to develop their skills including (i) contentdriven team interactions within the Competence Areas and the Translational Research Teams, (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 (Universities of California, Tsinghua, Melbourne University, and universities of our cooperation partners). FSC encourages their Ph.D. students to also supervise smaller projects together with B.Sc. and M.Sc. students in order to develop leadership skills. Scientific cooperation and team work will further knit a strong network between the early career researchers. A strong scientific mentoring by two supervisors, where applicable from different disciplines, will be mandatory.

Postdoctoral Researchers: The end of the doctoral and the beginning of the postdoctoral phase represents an important transition phase towards academic independence. Own research achievements from the Ph.D. phase have been published, new independent scientific leads emerge during this phase. First independent academic contours develop, and contributions to project guidance, management, and additional fund raising are expected. Postdoctoral researchers are preferentially recruited form outside and will give new impulses and contribute additional competences. They are eligible to the skill development portfolio of the FSC Research School, as well as CPL. RWTH will offer funding opportunities to Postdocs where they can apply for first independent funding within RWTH-wide competitive Call for Proposals. Female postdoctoral researchers will be supported and encouraged to further pursue an academic career. Corresponding measures to reconcile career and family are important and explained in Section 4.2 (Equal Opportunity).

Junior Research Group Leaders: These outstanding researchers have received their Ph.D. degree, excelled during a postdoctoral position and develop towards independent project leaders. They are encouraged and supported through the Advanced Talents Program to acquire their own budget through prestigious grants (Emmy Noether, ERC Starting Grant, Helmholtz junior research group etc.) and other research projects, supported by a mentor within the FSC or the RWTH program. To foster excellence at this career level, it is important to provide time and freedom for their research, an attractive scientific environment and intellectually stimulating cooperations. Junior research group leaders will be involved in teaching and have the privilege to supervise doctorates. Within FSC, Junior Research Group Leaders co-supervise at least two Ph.D. projects together with a PI. Upon suggestion by FSC Steering Committee and based on a rigorous evaluation procedure within the Faculty, they can obtain the right to independently supervise and graduate Ph.D. students. The envisioned career path of Junior Research group leaders should lead them as most probable next step to an external appointment as professor. In summary, the qualification concept for early career researchers within the FSC comprises:

- a research-related individualized FSC-specific curriculum with ample international networking and communication nodes,
- swift and effective integration into the FSC-teams (CAs and TRTs),
- regular scientific mentoring by PIs of the Cluster of Excellence including career advising and training,
- training regarding professional skills, scientific integrity, teaching, research data management, responsible research and innovation, and interdisciplinary research (CDS and CPL),
- the RWTH Seed Fund program to support independent research work of postdoctoral researchers and junior group leaders.

Tenure Track Program

The CoE TMFB has been actively shaping the research directions at faculty level. It also has been facilitating, paving, and shaping the current RWTH tenure track career path contributing to a formalized process. In 2017, RWTH has formally agreed upon a university-wide tenure track program. The overarching RWTH tenure track regulations are currently implemented in procedures and operational details by the faculties and will be effective by the time the FSC will start hiring tenure track candidates.

TMFB has used substantial funding for the support of junior research groups and junior professorships with tenure track option. Candidates understood the CoE as a facilitating means to develop their academic profile and progress from there and these positions have allowed early career researchers to develop from creative scientists to leaders in their field. They moved on to a professorship in the US (Ismael), a leading position at a governmental research institution (Physikalisch-Technische Bundesanstalt, Fernandez), a Reader position at Imperial College (Rinaldi), a Professor Position at TU Braunschweig (Schallmey), and as Director of a Leibniz Institute in Jena (Agler-Rosenbaum). One position has turned into a tenured position at RWTH already (Klankermayer). One candidate is close to his final evaluation, after successfully passing mid-term evaluation (Heufer). The latter two researchers are today PIs of the FSC.

FSC will significantly influence the research landscape of the involved faculties through its ambitious early career and tenure track goals. FSC incorporates one current tenure track candidate (Heufer) into its research program and initiates 11 new positions for tenure track- and Full-professorships (see Table 5.2.2).

In summary:

- FSC utilizes the scientific environment, infrastructure, and financial resources to substantially facilitate the development of the 11 new faculty members in their individual and independent research profile.

- For all positions planned at this stage, scenarios to sustain the position beyond the tenure track period are already agreed upon with the respective Faculties and the strategic partners of FZJ and MPI CEC.

- The opportunity to access the extensive existing infrastructure of FSC-PIs will permit a swift start for each new appointed faculty.

- Through its integrative research program structure and mentoring activities, the early career researchers will be able to quickly establish and expand their scientific network.

Early Career Coordination and Funding

A Steering Committee member (Wessling) is responsible for the management of the FSC 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 (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).

Kooperationen

Collaboration

The principal investigators of the "Fuels Science Center 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, is 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 is the exchange of students and researchers in the fields of catalysis and NMR science. While this program expires, FSC will maintain 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".
- In the area of biorenewable-based energy engineering, the University of Alberta (UAlberta) has been awarded the Future Energy Systems research initiative as part of Canada's First Research Excellence Fund competition - the excellence initiative of the Canadian government. RWTH and UAlberta currently establish an institutional partnership and intensify the cooperation on the basis of joint research projects, student and doctoral student mobility, collaboration for jointly planned and delivered courses, and mutual research and teaching visits of professors.
- The Undergraduate Research Opportunities Program UROP will offer specific research summerschools and internships at FSC research facilities. This program is well established and mostly brings students from North America to Aachen.
- With "CatchBio", a governmentally funded research network located in the Netherlands, TMFB has established an intense cooperation that will be continued between FSC and the "Netherlands Center for Multiscale Catalytic Energy Conversion".
- With e-Refinery and VoltaChem in the Netherlands, FSC has agreed to develop an annual exchange meeting comparable to the CatchBio cooperation.
- The Co-Optimization of Fuels & Engines (Co-Optima) initiative, a research and development (R&D) collaboration between the U.S. Department of Energy (DOE), nine national laboratories, and universities supports collaboration with the FSC to further its mission focused on developing a fundamental scientific understanding of approaches for improving the efficiency and reducing emissions of future propulsion systems.
- The Germany Ministry for Education and Research has established the so-called "Kopernikus Projects for Energy Transition" as major nation-wide networks of academic and industrial partners. One of them, Power-To-X, is coordinated by the FSC PIs Leitner (RWTH) and Eichel (FZJ) together with DECHEMA. Complementary to the FSC approach, the project focuses on the chemical storage and utilization of excess power by a combination of (co-)electrolysis and subsequent conversion of hydrogen, carbon monoxide, and synthesis gas with largely established catalytic processes. In the project SynErgie, directed towards

demand side management in production and manufacturing processes, one of the project areas (chemical processes) is headed by FSC PI Mitsos (RWTH).

- The “CAT Catalytic Center is a long-term strategic collaboration between RWTH and the company Covestro. With its already ten years of history and a current personnel of approximately 25 young researchers and technicians, it provides a successful example for translational research in public private partnerships. The fundamental research on catalytic CO2 conversion has been pivotal to the industrial implementation of a new industrial process in the polyurethane industry.

- RWTH is also partner within the European Doctoral Program on “Sustainable Industrial Chemistry - SINCHEM hosted by the University of Bologna/Italy. SINCHEM develops collaborations between high level academic and industrial teams across Europe and promotes student mobility.

Internationalisierung

Position of FSC within the National and International Research Area

The challenges and opportunities associated with a transition of the energy system and the use of nonfossil raw materials has led to major research initiatives world-wide. Rooted in its unique profile, in the scientific progress, and in the collaborative structures developed within the Cluster of Excellence “Tailor-Made Fuels from Biomass (TMFB)”, RWTH and its partners are ideally positioned to establish the “Fuel Science Center as a national lighthouse and an internationally leading scientific environment in this highly competitive field. Targeting “fuels as central pivot to interconnect the energy, mobility, and chemistry sectors allows the definition of common goals and a coherent research strategy for scientists at all career levels with diverse, yet complementary and synergistic expertise. The strategic partnership between RWTH, FZJ, MPI KoFo, and MPI CEC provides an excellent infrastructure and a critical mass of leading scientists, capitalizing on the individual profiles of the institutions within the German scientific landscape.

While a number of research institutions world-wide focus on either the conversion of renewable energy into chemical storage materials or the development of alternative propulsion systems, the integration of both fuel production and propulsion systems in one common research framework is quite rare. Apart from the CoE TMFB, one of the very few large-scale initiatives embracing production and propulsion is the recently launched Co-Optima Initiative started by the US Department of Energy (DOE) in March 2016 [CO]. The initiative intends to “combine the previously independent areas of biofuels and combustion R&D, bringing together two DOE Office of Energy Efficiency & Renewable Energy research offices, nine national laboratories, and numerous industry and academic partners to more rapidly identify commercially viable solutions [COa]. Current publications from this program deal mainly with the assessment of biomass-derived blending components for compatibility with existing engine concepts, infrastructures, and production routes [Du17]. The Co-Optima consortium has already indicated a strong interest to enter into collaboration with FSC in case of its approval.

The potential for a pivotal international position of FSC in this research area is demonstrated inter alia by its strategic links to major research institutions and scientific partners through its Scientific Advisory Board (see Section 4.3). This includes the Joint BioEnergy Institute (JBEI; San Francisco, USA) [BE], the Sustainable Energies Program at the Dalian Institute of Chemical Physics (Chinese Academy of Sciences, Dalian, China) [DICP], the Netherlands Center for Multiscale Catalytic Energy Conversion [MCEC], the Engine Research Center at the University of Wisconsin (Madison, USA) [ERC], the Center for Sustainable Chemistry at University of Nottingham (UK) [CSC], and the Center for Process Systems Engineering at Imperial College (London, UK) [PSE].

Based on the fundamental insight and methodological progress, FSC is able to act as a motor for translational research activities transferring knowledge into innovation. In addition to focused industrial projects aiming at implementation, this is exemplified in particular by coordinating roles in large scale national academic-industrial networks such as the Kopernikus project “Power-to-X and the BMBF initiative “Carbon2Chem®”. It is also reflected by the strong commitment of representatives from companies covering the entire value chain from energy systems to car manufacturers in the International Advisory Board (see Section 4.3.1).

Digitalisierung

Nachhaltigkeit (Niklas von der Aßen

Forschungsdatenmanagement (Herres-Pawlis / Dörte Rother)

Research Data Management(Herres-Pawlis / Dörte Rother)

FSC will define, support, and maintain standards for Research Data Management (RDM) within the cluster, but will also contribute to extending RDM methods, processes, and tools, and tailor these for the specific needs of the cluster. Within FSC, this should lead to a culture, where RDM is an integral, automated, and indispensable part of the complete data life cycle and scientific collaboration. FSC will implement the FAIR principles (Find, Access, Interoperate, and Re-use) of scientific data management and support open access as important cornerstones of good scientific practice. RDM will also be an important part of the annual internal peer project evaluation as described in section 4.3.3.

Within the first year of the project, FSC will establish a first version of a data management policy in accordance with principles of scientific data management of the participating institutions RWTH, FZJ, and MPI, which will be further extended during the course of the project. This process will be facilitated by the newly founded JARA-Center for Simulation and Data Sciences, the RWTH IT Center, and the RWTH University Library within the research data management efforts of RWTH described in the RWTH Strategy 2030. The policy includes data management plans specifically developed for the different research areas within FSC, details about appropriate meta-data schemata, and guidelines regarding institutional archiving, presentation platforms, and specialized repositories.

The RDM-responsible member of the FSC Steering Committee (Pitsch) together with a scientific data manager (SDM) will be responsible to coordinate the RDM activities within the FSC. The SDM will be a newly established position of a researcher at the interface of engineering, the natural sciences, and information technology co-supervised by one of the FSC PIs and the director of RWTH's IT Center. The SDM will ensure the proper identification and processing of data assets according to the data management policy. Responsibilities of the SDM include the promotion of open access and providing training and technical assistance to scientists. The SDM will further collaborate with the RWTH IT Center staff and FSC researchers (i) to develop tailored data management plans to accommodate the vastly different needs of researchers within the cluster from kB to tens of TB; and (ii) to support, from a user's point of view, the integration of new RDM tools developed in community efforts or by the FSC participating institutions, such as the application "Laborjournal presently under development at MPI.

Data management plans will guide data management throughout the data life-cycle, such that data will be enriched with appropriate meta-data already during its generation and that at the appropriate times, access is granted to collaborating researchers within FSC and to the scientific community. PIDs (persistent identifier system by the European Persistent Identifier Consortium EPIC) will be used to track the data from acquisition to archiving, publishing, and enabling long-term open access. RWTH's institutional repository will provide an option for data storage; furthermore, its tools for meta-data management and the creation of data management plans as well as templates for institutional policies will be used.

Transfer

Guidelines for section 5.3:

Where the Cluster of Excellence uses, generates and/or processes data, please describe the overall plans and policies for the handling of research data, samples, research software and/or other material and objects, including statements about data security, rights management, licensing, and publication support. How are research data, samples and research software securely to be archived and curated? What kind of re-use will be encouraged, e.g. by means of licenses? Please describe the overall strategies for publishing the research output, including the reusability of data, material and research software.

Describe the provisions for research facilities and instrumentation as appropriate. How is the planned infrastructure of the Cluster of Excellence embedded in existing structures and research facilities (such as instrumentation facilities and research data infrastructures, publication platforms, code repositories)? Where applicable, you may refer to central measures and resources provided by the applicant university/universities and participating institutions relating to data and information management as described in section 6.2 (e.g. data stewards, IT centres, libraries, imaging and other facilities).

Renewal proposals only: Please refer to the strategies pursued and measures established in the first funding period.

Please summarise the requested funds for these measures using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table. “Instrumentation” refers to all instruments, software and other equipment costing more than 50,000 euros per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 4 pages for this section.

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

Research data management

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. The previous cluster established a supporting structure with a data steward team. The team supported researchers by defining RDM standards, explaining the Findable, Accessible, Interoperable, Reusable (FAIR) principles [211] (see Table 5.3.1), and supporting in the development of tailored data management plans.
However, the efforts also showed that researchers in the cluster often have difficulties with starting and with knowing what is necessary for performing RDM. The number of tools available can be confusing and researchers struggle on the question on how to start RDM. This start includes choosing the right tools for RDM as well as the decision on what data to save and in which way. These are struggles that also researchers outside the clusters have [212][3–4]. To improve the RDM capabilities and support the researchers, 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. This will ultimately support researches in their decision making process on RDM approaches and therefore accelerate research progress within FSC.
Our initial RDM concept aims to facilitate RDM for researchers in the cluster and further develop the cluster's platform as a single point of access (see Figure 40). As the platform is already well-known and used by the researchers, the barrier to use it for additional activities as RDM is expected to be low. The access will be designed as a research data interface that collects relevant information about the data the researcher wants to manage. Additionally, the platform will connect to external services as RDM recommendation systems and RDM tools. Via this interface, researchers can get support in their decisions on which RDM tool to use and on setting up the required information in the chosen RDM tool.

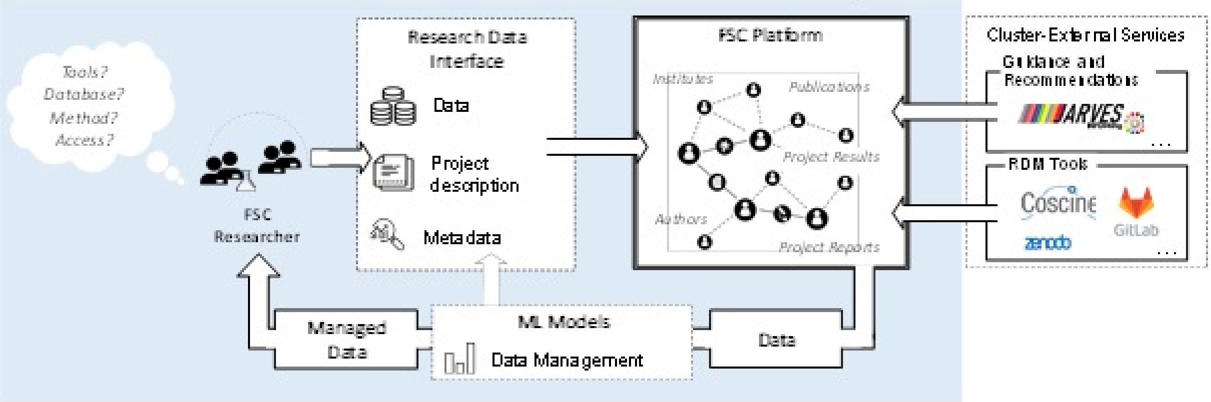

Figure 40: RDM concept within the cluster's platform.

Additionally, the concept aims to support the researchers in preparing data, as this is a necessary step for RDM. Effective data preparation is essential for ensuring data quality and accessibility throughout the research lifecycle. The management of data can be supported by utilizing ML models for organizing, cleaning, and anonymizing data. By providing support for managing the data, the barrier to use the RDM tools suggested by the external recommendation service is supposedly smaller. The models must be developed and deployed for the researchers in the cluster.

The proposed concept should also enable and promote RDM with the cluster according to the FAIR principles, as explained in Table 5.3.1.

Table 5.3.1: FAIR principles for RDM concept.

Findable	Connecting the chosen RDM tool with the project description makes the data easily findable for all cluster researchers. The use of the recommendation systems helps defining the user how to make the data findable for everyone in the research community, e.g., by publishing a data publication.
Accessible	The use of the RDM tools enables a way of storing data in a way that it is open to everyone.
Interoperable	The recommendation system helps in defining what is necessary for the specific data. The researcher can then choose the suitable managing ML model to support preparing the data to be easily integrated and exchangeable between different systems.
Reusable	The managing ML models help preparing the data in a way that other researchers can use it.

Data Management Coordination and Funding: The effort will be around 1 scientific researcher plus student support

Table 5.3.2: 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							
Direct project costs (excluding staff)							
Instrumentation							

Guidelines for section 5.4:

Describe the internal organisation and management structure of the Cluster of Excellence. Detail the internal decision-making criteria and structures for central aspects such as internal allocation of funds and staff selection. Describe the Cluster's strategies for quality assurance (e.g. monitoring, evaluation etc.).

Explain how the Cluster of Excellence is institutionally integrated in the applicant university/universities and, if applicable, outline the collaboration with the participating institutions (cf. section 1.4).

Renewal proposals only: Please refer to the internal management structure of the first funding period. If applicable, please explain adjustments planned for the second funding period.

Please summarise the requested funds for these measures using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table. "Instrumentation" refers to all instruments, software and other equipment costing more than 50,000 euros per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 3 pages for this section.

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

RWTH Aachen University (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 Cluster of Excellences (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 Forschungszentrum Jülich (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 Max Planck Institute for Chemical Energy Conversion (MPI CEC). All collaborations within the The Integrated Fuel & Chemical Science Center (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 41. It continues the current operational management structure of FSC that has proven to facilitate both an effective and efficient co-ordination within the cluster and the continuous development and implementation of the strategic vision of the CoE. The Operational Cluster Management consists of three pillars: the Steering Committee, the International Advisory Board (IAB), and the Cluster Office.

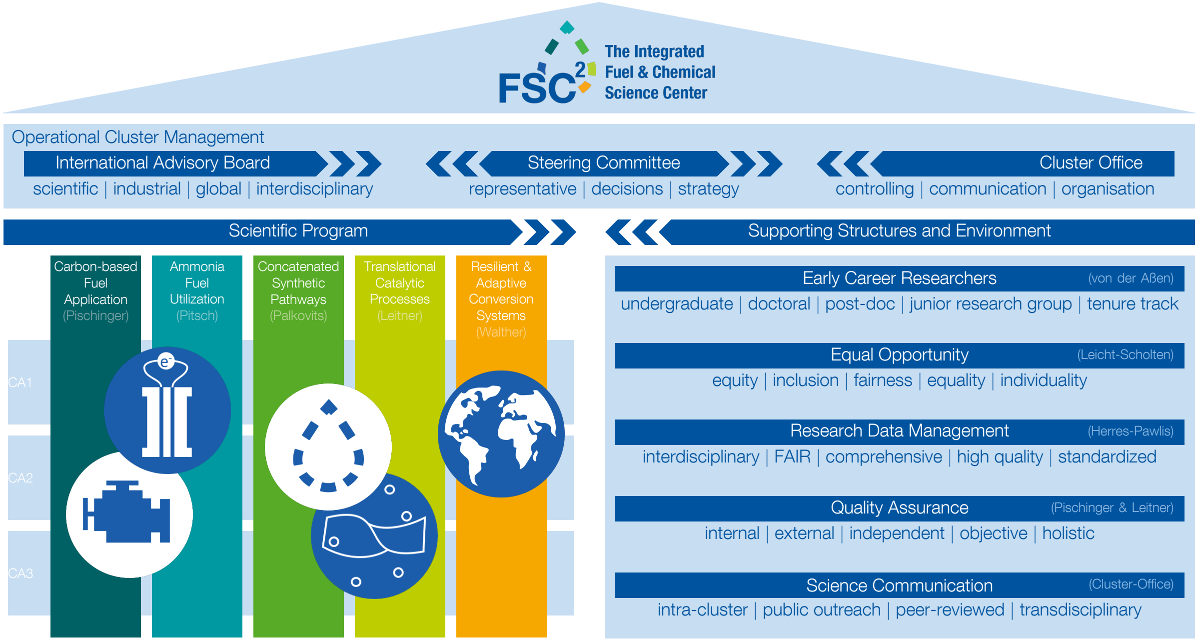

Figure 41: Management structure of the CoE

The Steering Committee is the central supervisory and decision-making board. The Steering Committee meets monthly. It is in charge of monitoring and steering all activities of the Scientific Program and the Supporting Structure. The Steering Committee is directed by the CoE's spokespersons Stefan 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 41). MPI CEC and FZJ are represented by Walter Leitner and Regina Palkovits, respectively. Those responsible for the measures of the Supporting Structure report to the Steering Committee on a monthly basis and as required.

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. Joachim Damasky	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
Dr. Charles Westbrook	University of California	Combustion Chemistry
Prof. Tao Zhang	Dalian Institute of Chemical Phsysics	Director

The Cluster Office consists of a Chief Operating Officer (COO) and a Chief Financial Officer (CFO) who are appointed by the coordinator of the CoE. The COO manages and supports the Steering Committee in assessing the scientific progress as well as the alignment of the individual projects to the interdisciplinary research goals of 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 Competence Areas (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 Translational Research Teams (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

Table 5.4.1: Caption

valued[1].

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.

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							
Direct project costs (excluding staff)							
Instrumentation							

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

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

Guidelines for section 5.5:
Please explain what strategies are envisaged for science communication. What strategies or techniques will the Cluster of Excellence use to communicate its research objectives, approaches and findings to specific target audiences and/or the lay public? How will the transfer of knowledge be organised? Where applicable, please outline any plans to incorporate research-oriented teaching.

Renewal proposals only: If applicable, please refer to relevant strategies and achievements of the first funding period.

Please summarise the requested funds for these measures using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table. “Instrumentation” refers to all instruments, software and other equipment costing more than 50,000 euro per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 3 pages for this section.

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 Mattermost), in which teams organize themselves according to the CAs, TRTs, and situational communication teams.

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							
Direct project costs (excluding staff)							
Instrumentation							

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

Guidelines for section 6.1:
Please comment on the suitability of the applicant university/universities and what role the Cluster of Excellence will play in its/their proposed structural development. Outline its/their priorities, also with regard to the overall strategic concept(s) of the institution(s), including projects already funded through the Excellence Strategy and/or other proposals.
In case of a joint proposal, the cooperation between the applicant universities and the academic and structural benefits it offers should be described for each of the applicant universities.
Renewal proposals only: Please describe the relevant achievements of the first funding period.

Estimation: In total, a maximum of 2 pages for this section.

6 Environment of the Cluster of Excellence

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

Guidelines for section 6.2:

Please explain what contribution each applicant university and participating institution is currently providing and will provide in the future in terms of staff, funding and infrastructure to support the Cluster of Excellence. Describe how this contribution is embedded in the strategic planning of the university/universities, for example in relation to existing and/or planned core research facilities (such as platforms, research data infrastructures, publication platforms, code repositories). Where necessary and appropriate, reference should also be made to strategies and access policies relating to key technologies and IT.

Estimation: In total, a maximum of 2 pages for this section.

Table 6.2.1: New tenure track positions and lighthouse appointments generated within the FSC[2]

6.2 Resources provided by the institution(s)

Guidelines for section 6.3:

Please describe the existing and planned collaborations between the Cluster of Excellence and other institutions both in Germany and in other countries.

Please summarise the requested funds for collaborations using the table below, and provide a justification for your request in the text. Note that staff funding requested as part of the research programme in section 4.5 should not be included in this table. “Instrumentation” refers to all instruments, software and other equipment costing more than 50,000 euros per item. Instrumentation costing more than 150,000 euros per item should be listed individually.

Estimation: In total, a maximum of 2 pages for this section.

6.3 Collaboration with external partners

The principal investigators of the “Fuels Science Center” 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, is 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 is the exchange of students and researchers in the fields of catalysis and NMR science. While this program expires, FSC will maintain 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”.
- In the area of biorenewable-based energy engineering, the University of Alberta (UAlberta) has been awarded the Future Energy Systems research initiative as part of Canada’s First Research Excellence Fund competition - the excellence initiative of the Canadian government. RWTH and UAlberta currently establish an institutional partnership and intensify the cooperation on the basis of joint research projects, student and doctoral student mobility, collaboration for jointly planned and delivered courses, and mutual research and teaching visits of professors.
- The Undergraduate Research Opportunities Program UROP will offer specific research summerschools and internships at FSC research facilities. This program is well established and mostly brings students from North America to Aachen.
- With “CatchBio”, a governmentally funded research network located in the Netherlands, TMFB has established an intense cooperation that will be continued between FSC and the “Netherlands Center for Multiscale Catalytic Energy Conversion”.
- With e-Refinery and VoltaChem in the Netherlands, FSC has agreed to develop an annual exchange meeting comparable to the CatchBio cooperation.
- The Germany Ministry for Education and Research has established the so-called ”Kopernikus Projects for Energy Transition” as major nation-wide networks of academic and industrial partners. One of them, Power-To-X, is coordinated by the FSC PIs Leitner (RWTH) and Eichel (FZJ) together with DECHEMA. Complementary to the FSC approach, the project focuses on the chemi-cal storage and utilization of excess power by a combination of (co-)electrolysis and subsequent conversion of hydrogen, carbon monoxide, and synthesis gas with largely established catalytic processes. In the project SynErgie, directed towards demand side management in production and manufacturing processes, one of the project areas (chemical processes) is headed by FSC PI Mitsos (RWTH).
- The “CAT Catalytic Center” is a long-term strategic collaboration between RWTH and the compa-ny Covestro. With its already ten years of history and a current personnel of approximately 25 young researchers and technicians, it provides a successful example for translational research in public private partnerships. The fundamental research on catalytic CO2 conversion has been pivotal to the industrial implementation of a new industrial process in the polyurethane industry.
- RWTH is also partner within the European Doctoral Program on “Sustainable Industrial Chem-

istry – SINCHEM" hosted by the University of Bologna/Italy. SINCHEM develops collaborations between high level academic and industrial teams across Europe and promotes student mobility.

- refuel.ch, ETH Zürich.
- BioSC?
- Aufbrauch (Rother)
- etos (Waldvogel)
- Hydriogeni, Norwegen (Pitsch)
- NEDO, Japan (Pitsch)

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							
Direct project costs (excluding staff)							
Instrumentation							

Guidelines for chapter 7:

In this section the funds requested in sections 4, 5 and 6 above are summarised according to various aspects. Please complete the following table to show the amount of funding requested for the subunits of the proposed research programme.

In table 7.1, please summarise the amount of funding required to implement the Cluster's Research Programme broken down to the research subunits and cost types, as described in section 4.5. "Instrumentation" refers to all instruments, software and other equipment costing more than 50,000 euros per item.

In table 7.2, please summarise the amount of funding required to implement the Cluster's structural measures (from sections 5 and 6). The measures listed are examples and can be modified, added to or omitted as necessary.

In table 7.3, please list the number of staff positions requested for the Cluster of Excellence.

In table 7.4, list the respective total amounts of funding requested for the Cluster of Excellence overall – not including the programme allowance for indirect project costs and the university allowance – broken down by funding category and year. Again, "Instrumentation" refers to all instruments, software and other equipment costing more than 50,000 euros per item.

Estimation: In total, 2 pages for this chapter.

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