The Integrated Fuel & Chemical Science Center

Adaptive Conversion Systems for Sustainable Energy Carriers and Chemicals

Renewal Proposal EXC2186

Contents

Nomenclature

Acronyms and abbreviations

AI	artificial intelligence
AR	Associated Researcher
CA	Competence Area
CA1	Competence Area 1
CA2	Competence Area 2
CA3	Competence Area 3
COE	Cluster of Excellence
CTY	ChemTraYzer
DAC	direct air capture
DLFC	direct liquid fuel cell
EU	European Union
FAIR	Findable, Accessible, Interoperable, Reusable
FDP	Fuel Design Process
FSC	The Fuel Science Center
FSC^2	The Integrated Fuel & Chemical Science Center
FZJ	Forschungszentrum Jülich
GCMS	gas chromatography and mass spectrometry
GHG	greenhouse gas
HR	high reactivity
ICE	internal combustion engine
IDT	ignition delay time
LAS	laser absorption spectroscopy
LBV	laminar burning velocity
LCA	life-cycle assessment
LR	low reactivity
MCCS	molecularly controlled combustion system
MCPS	molecularly controlled propulsion system
MCR	multivariate curve resolution
MD	molecular dynamics
ML	machine learning
MPI CEC	Max Planck Institute for Chemical Energy Conversion
MS	molecular spark
MT	molecular torch

NLP	natural language processing
PI	Principal Investigator
PNFA	process network flux analysis
QM	quantum mechanics
RCM	rapid compression machine
RDM	research data management
RWTH	RWTH Aachen University
SDF	Systems Design Forum
SRA	Strategic Research Area
SRA-AC	Strategic Research Area – Ammonia Conversion
SRA-CBFC	Strategic Research Area – Carbon-based Fuel Conversion
SRA-CSP	Strategic Research Area – Concatenated Synthetic Pathways
SRA-RACS	Strategic Research Area – Resilient & Adaptive Conversion Systems
SRA-TCP	Strategic Research Area – Translational Catalytic Processes
ST	shock tube
TMFB	Tailor-Made Fuels from Biomass
TRT	Translational Research Team
UDE	universal differential equations

Symbols

η_i	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(s)	Institution
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/temporary [LB1]
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 [LB2]
6	Univ.-Prof. Dr. rer. nat. Sonja Herres-Pawlis	Aachen, RWTH	Chair of Bioinorganic Chemistry	W3/permanent
7	Prof. Dr.-Ing. Karl Alexander Heufer	Aachen, RWTH	Chair of High Pressure Gas Dynamics	W3/permanent
8	Univ.-Prof. Dr.-Ing. Andreas Jupke	Aachen, RWTH	Chair of Fluid Process Engineering	W3/permanent
9	Univ.-Prof. Dr. rer. nat. Jürgen Klankermayer	Aachen, RWTH	Institute of Technical and Macromolecular Chemistry (Translational Molecular Catalysis)	W3/permanent
10	Univ.-Prof. Dr. rer. nat. habil. Lars Lauterbach	Aachen, RWTH	Synthetic Microbiology Teaching and Research Area	W2/permanent
11	Univ.-Prof. Dr. rer. nat. Walter Leitner	Aachen, RWTH	Institute of Technical and Macromolecular Chemistry (Technical Chemistry and Petrochemistry)	W3/permanent
		Mühlheim a.d.R., MPI CEC	Chemical Energy Conversion	
12	Prof. Dr. techn. Karl Mayrhofer	Erlangen, FZJ	Helmholtz Institute Erlangen-Nürnberg for Renewable Energy	W3/permanent
13	Univ.-Prof. Dr. rer. nat. Anna Mechler	Aachen, RWTH	Chair of Electrochemical Reaction Engineering	W3/temporary
14	Univ.-Prof. Alexander Mitsos, Ph.D.	Aachen, RWTH	Chair of Process Systems Engineering	W3/permanent
		Jülich, FZJ	Energy Systems Engineering	
15	Univ.-Prof. Dr. rer. nat. Regina Palkovits	Aachen, RWTH	Institute of Technical and Macromolecular Chemistry (Heterogeneous Catalysis and Technical Chemistry)	W3/permanent
16	Univ.-Prof. Dr.-Ing. (USA) Stefan Pischinger	Aachen, RWTH	Chair of Thermodynamics of Mobile Energy Conversion Systems	W3/permanent
17	Univ.-Prof. Dr.-Ing. Heinz Pitsch	Aachen, RWTH	Institute for Combustion Technology	W3/permanent
18	Univ.-Prof. Dr. rer. nat. Dörte Rother	Jülich, FZJ	Institute of Bio- and Geosciences	W3/permanent
19	Univ.-Prof. Dr. Franziska Schoenebeck	Aachen, RWTH	Chair of Organic Chemistry I and Institute of Organic Chemistry	W3/permanent
20	Univ.-Prof. Dr. phil. Carmen Leicht-Scholten	Aachen, RWTH	Chair of Gender and Diversity in Engineering	W3/permanent

No.	Principal investigators	Location/Institution	Field of expertise	Position
21	Univ.-Prof. Dr. rer. nat. Ulrich Simon	Aachen, RWTH	Chair of Inorganic Chemistry and Electrochemistry	W3/permanent
22	Prof. Dr. Siegfried R. Waldvogel	Mühlheim a.d.R., MPI CEC	Chemical Energy Conversion	W3/permanent
23	Univ. Prof. Dr. rer. pol. Grit Walther	Aachen, RWTH	Chair of Operations Management	W3/permanent
24	Univ.-Prof. Dr.-Ing. Matthias Wessling	Aachen, RWTH	Chair of Chemical Process Engineering	W3/permanent
25	Univ.-Prof. Dr. rer. nat. Mirijam Zobel	Aachen, RWTH	Institute of Crystallography	W3/permanent

N principal investigators are women; this is a share of n percent.

1.6 Cooperation partners

No.	Institutional cooperation partners	Location
1	Yale University	USA
2	The University of Manchester	United Kingdom
3	Universidad de Valencia	Spain
4	Johann Wolfgang Goethe-Universität Frankfurt	Germany
5	Princeton University	USA
6	University of California	USA
7	The University of Nottingham	United Kingdom
8	King Abdullah University of Science and Technology	Saudi Arabia
9	Massachusetts Institute of Technology	USA
10	Utrecht University	The Netherlands
11	University of Alberta	Canada
12	University of California	USA

No.	Individuals as cooperation partners	Location
1	Paul Anastas	USA
2	Adisa Azapagic	United Kingdom
3	Avelino Corma	Spain
4	Henner Hollert	Germany
5	Yiguang Ju	USA
6	Jay Keasling	USA
7	Martyn Poliakoff	United Kingdom
8	S. Mani Sarathy	Saudi Arabia
9	Greg Stephanopoulos	USA
10	Bert Weckhuysen	The Netherlands
11	C. R. (Bob) Koch	Canada
12	Charles Westbrook	USA

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

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. 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 exceeding the gigantic production of 100 barrel per day 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 de-fossilization of the energy system imposes challenges and opportunities for the sectors mobility/transportation and chemistry where direct electrification is difficult or even impossible due to the indispensable need for carbon. Shaping a post-fossil area at the interface of energy and chemistry therefore requires novel research concepts and breakthroughs in fundamental science as basis for disruptive technologies that will result in major societal and economic transformations.

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

Vision

In the context of this dynamic development of utmost importance 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 (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 chemical energy carriers and products.

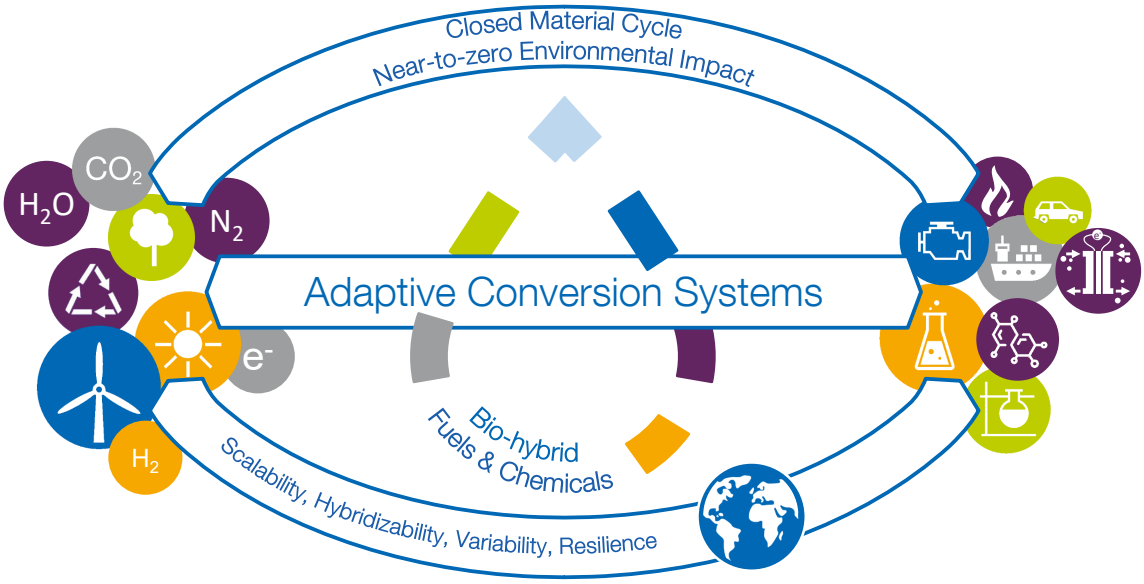

Figure 3.1: Vision of FSC^2 "The Integrated Fuel & Chemical Science Center generates fundamental knowledge and novel scientific methods for the development of adaptive technical solutions to valorize renewable electricity and feedstocks into liquid energy carriers and chemicals in a systems approach".

Mission

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 strategic development of projects and structural measures, a fundamental understanding of "fuel design" was successfully established for the first time. The subsequent COE, The Fuel Science Center (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.

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. All research activities and projects are allocated within Strategic Research Areas (SRAs) where they absorb and vice versa stimulate the disciplinary progress of the individual Principal Investigators (PIs), thus constantly augmenting the CAs. With the specific infrastructure of the partner institutions and the scientific profiles of the involved PIs, FSC^2 is ideally positioned to align groundbreaking science with focal technology options for post-fossil molecular energy carriers and products. Continuing efforts will be devoted to 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 thermal combustion, electro-chemical devices for recuperation of the chemical stored energy are being studied. The chemical value chain is addressed explicitly as major area of application for the novel synthetic pathways and catalytic processes. Analysis on a systems level is developed as integrative part to provide design criteria for sustainability and resilience.

Objectives

The SRAs for 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 conver-

sion 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 backward-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 integrated Fuel 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 efficiency and low emissions in thermochemical utilization. Solutions will be developed combining the molecular-torch concept with utilizing partial in-process reforming to hydrogen and innovations in exhaust-gas aftertreatment specifically for the very potent greenhouse gas N_2O.

- How can chemical, biochemical, and electrochemical transformations for the manipulation of C–O and C–N bonds be interlinked to open concatenated synthetic path-

ways 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 bio-catalysis. To establish effective connections between starting materials and desired molecular architectures, however, the transformation steps need to be designed and developed with a focus on the transfer points of intermediate products, reaction media and the recycling of the catalyst system from the beginning. Therefore, the selection of the most appropriate catalytic discipline is not determined solely by the evaluation of the individual catalytic transformation, but rather by the most efficient contribution within a transformation cascade of concatenated catalytic steps.

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

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. Over the first funding phase of FSC, we have increasingly utilized techniques from machine learning and their importance in FSC^2 will substantially grow. We use cutting-edge methods and contribute to their further development, mostly with funding external to FSC. We coordinate the activities around machine learning and ensure synergy among the different groups. A particular advantage of FSC for machine learning is that we generate own experimental data. Our research data management. Prominent examples of our activity are: data-driven and hybrid data-driven/mechanistic models for the prediction of properties that cannot be predicted fully mechanistically, e.g., for fuel combustion or life-cycle impact of production processes or catalyst performance; surrogate models for resource-efficient computation, e.g., within optimization of production processes using multi-scale modeling or within computational fluid dynamics; machine learning-enhanced decisions, e.g., Bayesian hardware-in-the-loop optimization or solvent design using variational autoencoders.

Structure
-Connection to JARA-CSD, AICenter: RWTH has network that will allow FSC to blossom
-Training of doctoral researchers on ML
-Dedicated excahnge platform on ML
-Research data management will become more important, especially for ML
-Connect to NFDI

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

- introduction bio-hybrid fuels
- fuel design process?
- 3 Storys?
- Cyclic Acetals –> Bio-hybrid Fuel Synthesis
- HyFiT /Methylketone
- EEBC–> KEAA –> Balanced FSC Blend
- Molecularly Torch & Spark?

The most promising bio-hybrid fuel candidates identified in FSC's iterative fuel design process 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 biohybrid 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 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.
from HyFiT abstract: Synthetic fuels are promising for sustainable transport. However, the current synthetic fuel options are either not suitable for the current fleet of vehicles or require new production processes, which has delayed their introduction to the market. A potential solution is the use of Hydroformylated Fischer-Tropsch (HyFiT) fuels. This fuel option combines two established technologies, Fischer-Tropsch synthesis and hydroformylation, to create a mixture of alkanes and alcohols that can serve as fuel. The goal of HyFiT-fuels is to address four main challenges of synthetic fuels: (1) using mature technologies, (2) compatibility with global fuel standards and elastomer materials, (3) reducing combustion-induced emissions, such as NO_X and particulate matter (PM), and (4) supporting the transition to net-zero greenhouse gas emissions. The research conducted shows that HyFiT-fuels can effectively tackle all of these challenges simultaneously, and therefore, offer a promising complement to electrification efforts. The investigations reveal 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. The study experimentally examines the fuel's impact on the emissions of CO_2, PM, and NO_X, and the theoretical potential for NO_X reduction by increasing exhaust gas recirculation (EGR) rates. The results show that HyFiT-fuels used as drop-in fuel without any further adaptations can reduce PM engine-out emissions by 55% (HyFiT-20%) respectively 70% (HyFiT-40%) and CO_2 tailpipe emissions by 3-5% compared to diesel fuel.

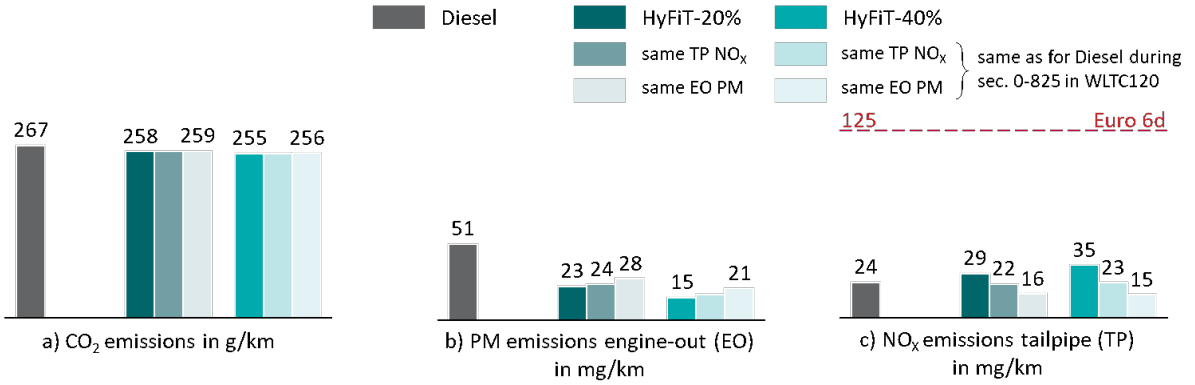

Figure 4.1: cumulative a) carbon dioxide (CO_2), b) particulate matter (PM) and c) NO_X emissions during WLTC120 of Diesel, HyFiT-20% and HyFiT-40% fuel with optimized calibration for emission reduction

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.

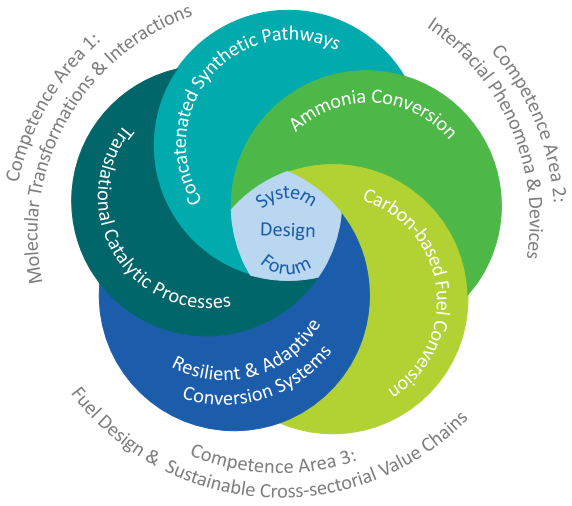

Figure 4.2: The integrated framework of the five Strategic Research Areas (SRAs) embedded within the Competence Areas (CAs).

4.3 Structure of the research program

- current CA Structure –> pool of expertise to address the ”big Challenges” –> adaptive research structure
- SRA

The SRAs are bridged via general design challenges that will be addressed in flexible working groups as the research program develops. This includes for example the integration of production pathways and propulsion properties for the C-based fuel design, the fundamental mechanisms of electro-chemical 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. A common platform for the scientific exchange and continuous adjustment of the overall research program in light of its mission and vision is provided in the Systems Design Forum (SDF), where the progress of the five SRAs and the working groups is biannually reported and discussed.

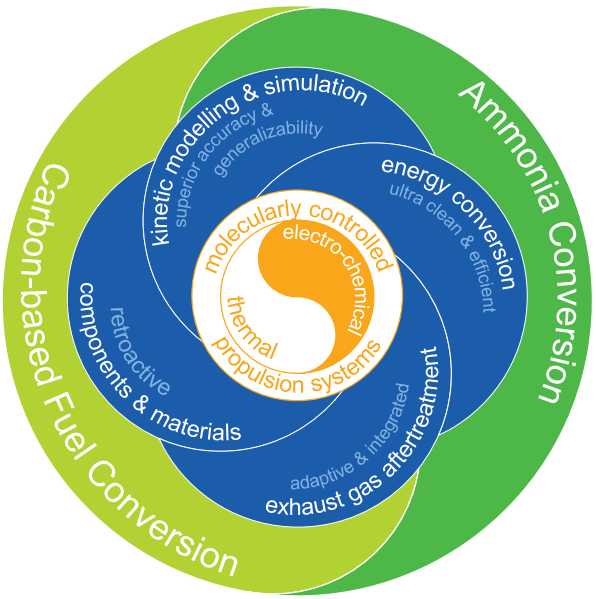

Figure 4.3: Joint methodologies and targets of Strategic Research Area – Carbon-based Fuel Conversion (SRA-CBFC) and Strategic Research Area – Ammonia Conversion (SRA-AC)

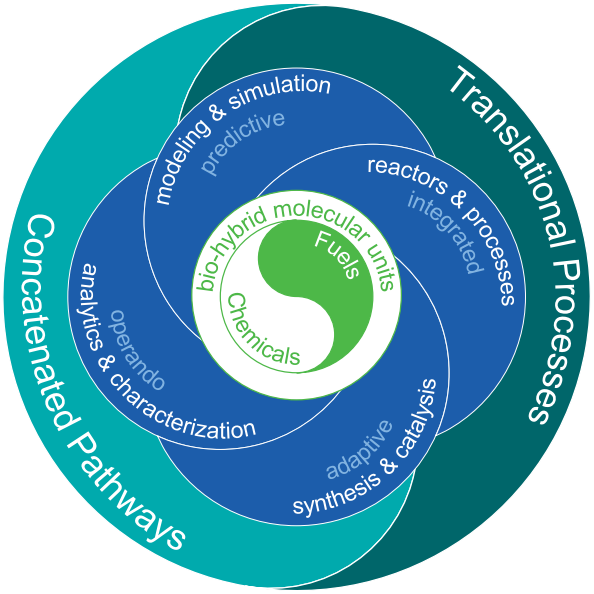

Figure 4.4: Joint methodologies and targets of Strategic Research Area – Concatenated Synthetic Pathways (SRA-CSP) and Strategic Research Area – Translational Catalytic Processes (SRA-TCP)

The 25 core PIs represent the three CAs and define the thematic focus within the SRAs. The project work is, however, based on a much larger network of scientific excellence and methodological expertise through about 15 associated PIs. All PIs have the same rights and responsibilities within the Cluster, creating the necessary critical mass and structural impact among the partner institutions. The resulting flexibility ensures continuing rejuvenation of the network of PIs including strategic appointments and early succession models. A major component is the support of early career academics opening new career paths across the institutional landscape.

Guidelines for section 4.4:
Outline the research profiles of the principal investigato
tigators, staff and the cooperating partners contribute t
objectives? Explain which other individuals and insti
will be involved in the future according to your current
investigators, staff, and cooperation partners, appropria
to diversity.
Renewal proposals only: Please include a concise synops
first funding period.

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

4.4 Staff and institutional composition of the Cluster of Excellence

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 Conversion

PIs: Pischinger (coordinator); Blank, Eichel, Heufer, Jupke, Klankermayer, Lauterbach, Leitner, Mechler, Mitsos, Pitsch. ARs: Boxx, Kneer, Leonhard, Magnus, Schmitz, Schröder.

How does the molecular structure of carbon-based fuels impact on efficiency and emissions upon recuperation of the chemically stored energy in retroactive and prospective molecularly controlled propulsion systems?
In the current phase, all degrees of freedom of bio-hybrid fuel molecules and molecularly controlled combustion systems (MCCSs) 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 integrated Fuel Design Process (FDP) established by FSC.

Strategy and Structure of SRA

The SRA "Carbon-based Fuel Conversion" 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 combustion processes and electro-chemical conversion at the molecular level (CA 1), as well as the associated energy conversion systems, internal combustion engines (ICEs), and direct liquid fuel cells (DLFCs) at the device level (CA 2). In line with the holistic, integrated FDP, the results contribute on 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 MCCS as well as high-performance and high-adaptivity aftertreatment systems in combination with bio-hybrid fuels to highly efficient and zero-impact emission molecularly controlled propulsion systems (MCPSs), introducing the concept of retroactive fuel and powertrain co-optimization.
Furthermore, with the new research field of DLFCs, electro-chemical energy conversion systems are integrated into the FDP to harness their potential for high thermal efficiency combined with high energy and power densities.

4.5.1.1 Retroactive Bio-hybrid Fuels XXX

The focus of the overarching optimization problem within the Fuel 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 retroactive thermal as well as prospective electro-chemical 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 Design Process. The in-depth understanding of the efficient energy conversion, emission formation and molecular interaction of retroactive, 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.

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, including many ML models, were successfully developed as part of FSC for prediction details of pyrolysis and oxidation behavior of fuels (P1, P2, P3, P4, P5, P6, P7, P8), Such developments base on a detailed theoretical calculation of molecular dynamics (MD) [Döntgen2015], of rate constants [Döntgen2018], and of thermodynamic data, as well as experimental results on laminar burning velocity (LBV) (P18), ignition delay times (IDTs) [H3], species measurements in flow reactors, and flame emissions (P9, P10) 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 (P11) and a comparative quantitative analysis of ammonia combustion models (P12) demonstrated how knowledge of complex oxidation processes can be consolidated. Other popular approaches are automatic model generation (P13, P14) and parameter estimation (P14).
The highly recognized FSC-tool ChemTraYzer (CTY) (reviewed by Dewyer2018, Simm2019, Miller2021) performs MD simulations to find new reaction pathways and obtains accu-

rate properties of the reactions by automated high-level quantum mechanics (QM) [Döntgen2015] [Döntgen2018] [Krep2023, Kopp2023, Schmalz2024].
However, achieving the ambitious goal of developing retroactive 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 X. 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 (P15, P16, P17), 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 [H5]. Owoyele and Pal [H6] 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 [H7] will be key to the further development of this method.

(kürzen, Abgleich Boxx?): 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 [H1-6]. For the species measurements, two different laser systems are being used. The 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: $fuel + \dot{O}H \Leftrightarrow fuelradicals + H_2O$, can be measured. The second laser system is an IR-laser that measures a wavenumber range of $60\,cm^{-1}$ with a time resolution of $4\,\mu s$. The currently used central wavenumber is $1740\,cm^{-1}$ and is able to measure the stretching of the carbonyl group, for example in formaldehyde [H11] or alkyl formats [H9]

but can be exchanged by other laser modules. 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 [H6-8]. For the GCMS measurements a sample needs to be taken from the reactive mixture in ST or RCM by fast opening valves (opening time: $1\,ms$) [H12]. 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.

Ensuring the long-term material compatibility of bio-hybrid fuels with engine, fuel cell and infrastructure components is crucial for the successful integration of retroactive fuels into existing and prospective energy conversion systems. Immersion tests, as part of The Fuel Science Centers (FSCs)' comprehensive fuel investigations, revealed an critical [S1-S5] 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 [S6].
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

FSC^2 aims to devise and implement new numerical and experimental methods to determine the reaction network, thermodynamic as well as tribological properties, and process performance of bio-hybrid fuels and materials, e.g., seals and membranes, that facilitate an ML-assisted Fuel Design Process for both retroactive 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,
- extensive, 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 ultra low-emission operation conditions:

- a new analysis tool for complex multi-component spectra using a combination of QM and MCR aided with GCMS species measurements.
- a new rapid multi-sampling technique with significantly decreased sampling time to achieve high temporal resolution

In addition, ML-based numerical and accelerated experimental methods for predicting the long-term durability of seals and materials are to be developed, particularly with regard to the compatibility of retroactive propulsion systems within the existing fleet.

Work program

from Pitsch_CBFC:

- Curation of an extensive database building on existing high-quality data from previously developed chemical kinetic models
- Use of NLP and other deep learning techniques, and reinforcement learning with established cheminformatics techniques (Tanimoto similarity of reaction fingerprints), methods from kinetic model reduction (DRGEP [24]), and sensitivity analysis (adjoint sensitivity analysis [25])

from Leonhard_TCP:

- When are physical models better and when ML? How can CTY help in the development of active learning ML algorithms? How to most efficiently design molecules based on QM and ML methods?
- How to include complex reaction networks (stability and catalysis) into the design efficiently?
- How to integrate “the big picture” into design (models from EHS (Environment, Health and Safety, LCA (Life-Cycle-Analysis))?

from Schmitz_CBFC:

- Application of machine learning classification based on the molecular character of fuels and sealing materials for the prediction of compatibility
- Implementation of EHL-simulations of dynamic seals for the evaluation of tribological properties and long-term behavior as well as for the modeling of fuel intake via piston rings
- Development of fast-EHL algorithms to reduce simulation time [12]
- Long-term immersion tests, tribological experiments and determination of fluid physical properties with existing measurement infrastructure (automated immersion test bench, drop-shape analyzer, densitometer, tensiometer, viscometer)

Pischinger

4.5.1.2 Retroactive Engine & Exhaust Gas Aftertreatment Design

The highly adaptive design of molecularly controlled propulsion systems is developed along a multi-stage, retroactive efficiency walk, which exploits the potential of the retroactive 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 aftertreatment systems. In addition to material compatibility, the conversion of pollutant emissions from ultra-lean combustion processes in the exhaust gas aftertreatment system, in particular NO_X, is closely linked to the research questions in context of ammonia conversion (SRA-AC) as well as DLFC.
Within the Fuel Design Process, the propulsion system design is already inherently coupled to the LCA. In the context of retroactive fuel, engine and exhaust 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).

Previous work

In FSC, the potential of bio-hybrid fuels (neat and as blends) in combination with MCCS was unveiled. The co-optimization of engine and fuel enabled increases of the compression ratio, optimizations of the injector calibrations, and the implementation of ultra-lean molecular spark (MS) as well as molecular torch (MT) combustion concepts using a high reactivity (HR) fuel and a low reactivity (LR) one [1–10]. In this way, continuous increases of the engine's η_i up to 49.1% and reductions of the engine-out emissions (indicted specific NO_X emissions down to 0.1 g/kWh) were achieved (see figure 4.5).

- molecular spark & molecular torch (TME, ITV, WSA)

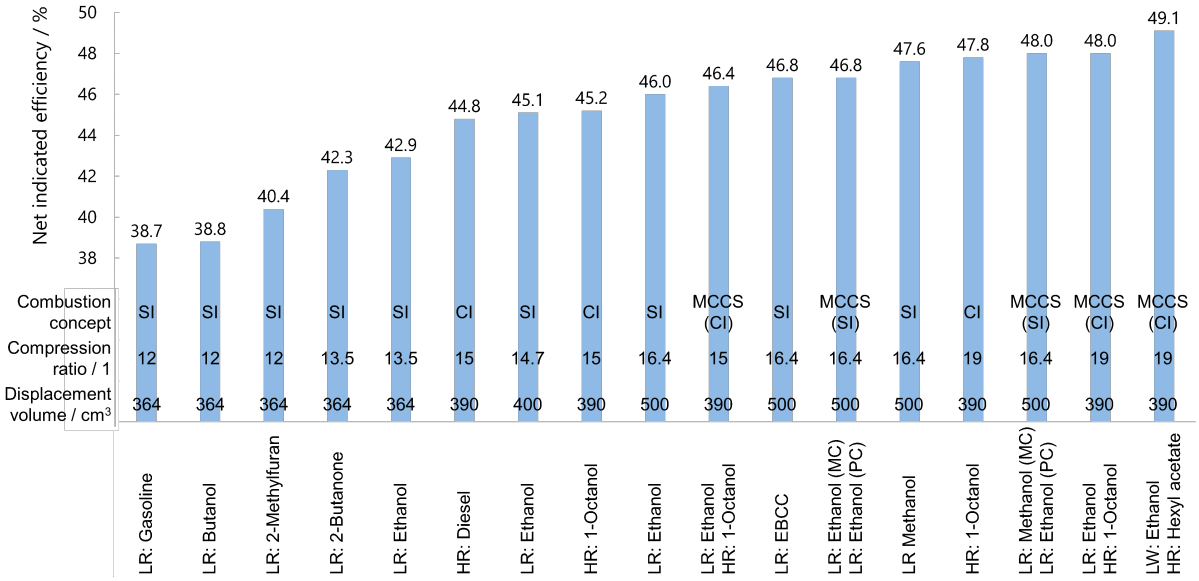

Figure 4.5: Efficiency Walk including molecularly controlled combustion systems

- numerical optimisation (AIA)
- exhaust aftertreatment (TME, IAC, ITMC, Modes, CVT)

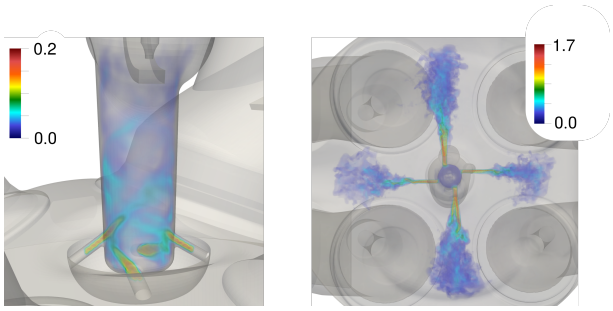

Figure 4.6: Volume rendering of the kinetic energy E of the ensemble-averaged flow field in the pre-chamber at 20°CA BTDC (left). Volume rendered instantaneous flow field of the gas jets into the main chamber at 1°CA BTDC (right)

Objectives

The concept of retroactive fuel and engine co-optimization is clustered in the multi-stage retroactive 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 fuels or fuel blends identified via the FDP implemented with correspondingly stringent constraints that ensure retroactive 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 FSC 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 exhaust gas recirculation (EGR) and optimized exhaust gas aftertreatment strategies. In the third stage, moderate hardware adaptations shall be considered. In particular, adaptations of the fuel supply system with respect to the injection pressure as well as of the injection system in terms of the mass flow rate are proposed to extend the engine operating range. In the final stage, the advanced molecular controlled combustion systems, molecular torch and molecular spark, discovered in FSC are to be implemented under the stringent boundary conditions of retroactivity. This involves hardware adaptations such as the implementation a high compression ratio piston in combination with a pre-chamber and a dual-fuel injection system as well as an advanced exhaust gas aftertreatment system.

- Development of retroactive fuel and engine co-optimization. retroactive bio-hybrid fuels shall be co-developed with a highly adaptive molecularly controlled propulsion system design, yielding an indicated efficiency of >50% for on-road passenger car engines.

- Development of a zero-impact emission strategy by combining the molecularly controlled propulsion system with a tailored exhaust gas aftertreatment system.

Work program

Mechler?/ Mayrhofer?

4.5.1.3 Organic Fuel Cells

Add short summary here.

Carbon-Based Liquid Fuel Cells

Abstract:

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 term 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. Here, we focus on the one hand on the "classical" fuels like alcohols and formic acid, but also explore more exotic versions like glycerol, urea, or ammonia-borane type fuel cells. 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. Furthermore, classical membrane fuel cells will be compared to biological fuel cells to allow for different use cases. 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 fuel design 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.

Goals:

- Development of components and full cells for different fuel types
- Characterizing systems for their flexibility in use of different fuels
- Reducing FC costs by reducing noble-metal utilization, improved efficiency and decreased cross-over & poisoning
- Use of designed fuels to improve sustainability and conversion efficiencies

Previous work

Objectives

Work program

Table 4.1: Proposed Staff in Research Subunit x

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

Table 4.2: Funding Request for Research Subunit x

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
Staff (Total for 4.5.x)							
Direct project costs (excluding staff)							
Total instrumentation < €150,000							
Total instrumentation > €150,000							
Instrument I > €150,000							
Instrument II > €150,000							

4.5.2 Strategic Research Area – Ammonia Conversion

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

Add short summary of SRA here

The strategic research area "Ammonia Conversion" focuses on developing clean systems for thermochemical and electrochemical conversion of ammonia (NH_3) as a carbon-free energy carrier. Internal combustion engines for off-road applications and high- and low-temperature fuel cells are considered. The low reactivity and high fuel-nitrogen content of ammonia present specific challenges for ammonia combustion engines, including instability, low efficiency, and emissions of NO_x, N_2O, and fuel slip. Reactivity enhancement, tailored mixing and combustion concepts, as well as catalytic and thermal cylinder coatings will be holistically explored to improve ammonia engine efficiencies and reduce engine-out emissions. To address the critical aftertreatment of the complex exhaust gas mixture, non-noble metal catalysts for coupled deNO_x-SCR and N_2O decomposition, as well as N_2O reduction by NH_3, will be developed based on a combination of experiments and numerical simulations. The electrochemical conversion of ammonia 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. Proton conducting separators, degradation mechanisms, and new membrane materials will be investigated to mitigate these issues.

Strategy and Structure of SRA

max 1-1.5 pages.

- Introduction to ammonia as carbon-free energy carrier. 1 paragraph
- Thermochemical and electrochemical conversion. 1 paragraph
- Introduction of the SRA consisting of three subsections with Schematic (interactions, position in real process).

Pitsch

4.5.2.1 Ammonia combustion

Add short summary here.

The low reactivity and high fuel-nitrogen content of ammonia pose specific challenges for ammonia combustion engines, including instability, low thermal efficiency, and emissions of NO_x, N_2O, and unburned ammonia. Mitigating these issues is proposed through tailored on-board reforming of ammonia generating hydrogen as highly reactive co-fuel to enhance combustion and ammonia-specific targeted advanced combustion concepts. The first project phase successfully developed lean-burn bio-hybrid fuel concepts that faced challenges similar to ammonia-based combustion, including the molecular spark and torch ignition strategies, optimized cylinder flow, and catalytic and thermal coatings. Adapting and optimizing these concepts will be vital in facilitating ammonia-based combustion. Additionally, novel gas and liquid injection concepts and mixing strategies, such as ejectors and H_2-saturated NH_3 injection, as well as combustion concepts for ammonia-hydrogen blends, will be explored. Hydrogen in fuel blends can cause nonlinear combustion behavior due to its higher reactivity and faster molecular transport. This presents an opportunity to tailor ammonia-hydrogen blends and combustion concepts for different operating conditions. To understand the intricate coupling of injection, mixing, and combustion, high-fidelity simulations of multi-fuel injection processes, mixing, combustion of fuel blends, flame-wall interaction, and pollutant formation will be conducted. In addition, comprehensive experimental measurements will be performed to unveil the fluid dynamic interaction of ammonia mixtures with dissolved hydrogen in the injector nozzle-internal flow. Advanced laser spectroscopy will provide in-depth knowledge of the ammonia-hydrogen injection and mixing processes with air, localize pollutant formation, and quantify pollutant emissions in turbulent high-pressure combustion environments. Combining experimental and numerical methods will pave the way for physics-based and data-driven modeling, which will be applied in device and system-level experiments to optimize device design and operation, considering instability, efficiency, emissions, and sustainability.

Current State of Research and Previous work

For ammonia combustion engines, two major challenges prevail: (1) Inefficient and unstable combustion resulting from ammonia's low reactivity and slow flame propagation speed [170]. (2) Additional emissions stemming from the fuel-inherent nitrogen, such as NO_x and high global warming potential nitrous oxide (N_2O), and from flame quenching and incomplete NH_3 combustion at the cylinder walls, which leads to ammonia slip [135]. Technological and fuel-related advancements are required to foster stable combustion and near-zero emissions. The investigated concepts in the first project phase, which focus on optimizing of lean-burn concepts for bio-hybrid fuels such as molecularly controlled igni-

tion or catalytic and thermal coatings, provide a proficient toolkit for tailoring efficient and clean combustion concepts for ammonia engines.

In the first project phase, a high-tumble engine with molecularly controlled ignition was developed, allowing for a high compression ratio ($CR = 16$) [14, 15, 13]. This engine demonstrated no knock limitation, short burn duration, and high indicated efficiencies when fueled with methanol. This promising combustion concept holds particular relevance for ammonia, which exhibits a higher octane number (approximately 130) than methanol (109). Ammonia's high knock resistance and ability to mitigate unintended auto-ignition make it suitable for spark-ignition engines with high compression ratios and potential high efficiencies. In addition to the high-tumble engine, a molecularly controlled high-swirl combustion system, where a high-reactivity fuel ignites a low-reactive mixture, was demonstrated to achieve a net indicated efficiency of 49.1%, as shown in Fig. 4.7 [100]. This provides an alternative promising combustion concept for low-reactive ammonia facilitated with on-board reformed highly reactive hydrogen.

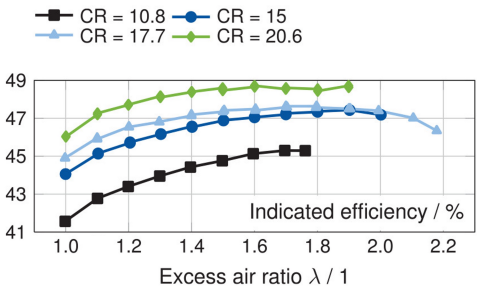

Figure 4.7: Effects of compression ratio and excess air ratio on the thermal efficiency of a methanol engine.

Detailed quantitative characterization of the individual in-cylinder processes and targeted injection strategies, in-cylinder flow, and ignition concepts are essential for engine development. This was achieved through a hierarchical approach, where the individual processes were studied on a subsystem level, such as broad parameter studies in various laminar and turbulent burners [121, 139, 141, 150, 149, 114, 122], the transparent automotive nozzle microscopy, combined with ultra-high-speed analysis of nozzle-internal two-phase flows [47], the flash-boiling analysis of superheated or evaporating droplet chains combined with 2-color LIF [55, 56], and the fuel-gas-solubility analyzer [39]. Multi-physics numerical simulation frameworks for spray, flash boiling, and combustion have been developed [67, 69, 68, 96, 7, 97, 22, 21].

A key challenge lies in further developing and optimizing established methods and exploring novel approaches for the combustion of ammonia and its blends with hydrogen. These fuels possess unique thermodynamic and combustion properties that differ significantly from conventional fuels, leading to distinct injection and mixing behavior, turbulence flame interactions, and pollutant formation. Consequently, tailored engine combustion concepts are necessary to address the specific challenges of ammonia engines. Prior investigations relevant to ammonia and hydrogen combustion have been conducted by the applicants, including studies on the chemical kinetics of ammonia and its blends with hydrogen [103, 32], ammonia flame speed measurement under microgravity conditions [33], catalytic ammonia reforming [74, 71], and hydrogen combustion under engine

conditions [19]. Furthermore, experimental and numerical investigations on Aerospike nozzles [92, 93, 30] and studies on the solubility of gases in liquids and the effects of dissolved gases on nozzle flow and spray break-up [1, 60, 61, 39] provide fundamental insights into designing promising mixing strategies for ammonia and hydrogen.

Objectives

The overall objective of the sub-SRA Ammonia combustion is to improve off-road ammonia engine efficiencies and reduce engine-out emission through targeted reactivity enhancement by on-board NH_3 reforming and accordingly tailored mixing and combustion concepts. The methods developed for bio-hybrid fuels during the first project phase will be further developed and optimized for ammonia, along with the introduction of novel gas and liquid injection concepts, mixing strategies with ejectors, and combustion concepts for ammonia-hydrogen blends. For this, it is critical to quantitatively characterize the flame propagation speed, turbulence flame interactions, and emission formation for both premixed and non-premixed combustion of ammonia and its blends with hydrogen. Another sub-objective is to design efficient catalysts for NH_3 reforming and to develop tailored strategies of injection, evaporation, and mixing for engine mixture preparation. The proposed novel approaches will be assessed and optimized in single-cylinder research engines. Particular emphasis will be placed on developing novel catalytically controlled and temperature-controlled pre-chamber ignition.

Work program

To comprehensively explore the potential for enhancing efficiency and mitigating engine-out emissions, a hierarchy of methods will be employed to investigate the intricate processes within the engine. This approach spans from fundamental analyses of individual processes to the optimization and analysis of devices and systems at various levels. To effectively utilize the specific combustion behavior of fuel blends with varying hydrogen content across different applications and operating conditions, it is crucial to quantitatively characterize the combustion behavior of ammonia. For this, various experimental facilities will be employed, such as turbulent compression reactor for high-pressure turbulent mixing, flame initiation, and propagation, as well as multi-functional burning chamber for high pressure turbulent jet flames (Pitsch). Further, single-shot 1D Raman spectroscopy and femtosecond 2-photon laser-induced fluorescence will be utilized to quantify the temperature and species during molecularly controlled mixing, ignition, and turbulent flame propagation in ammonia/hydrogen mixtures under high-pressure, high-temperature engine conditions. Specifically, the number density and distribution of important species, such as NH_3, NH, and atomic N, O, and H, will be determined (Boxx). In addition, high-fidelity DNS of molecularly controlled ignition of NH_3 and NH_3/H_2 and flame wall

interactions under engine conditions will be conducted (Pitsch), providing profound insights into complex nonlinear combustion behavior. This includes considering significantly different transport and chemical properties of the fuels, flame intrinsic instabilities, and intricate mixing and ignition processes during molecularly controlled ignition, enabling detailed analysis of turbulence interactions with chemistry, thorough examination of reaction pathways for pollutant formation, and development of high-fidelity LES models for device and system-level optimization.

To prepare tailored ammonia-hydrogen blends for different applications and operating conditions, investigations into both catalytic NH_3 reforming, either prior to or integrated into combustion, will be conducted (Palkovits). This involves employing a data-driven approach to design tailored high-entropy alloys and single-atom catalysts through combined high-throughput screening and machine learning-accelerated computational studies. A deep understanding of structure-activity relations will also provide insights into catalytic structures for NO_x/NH_3-slip abatement. Injection, evaporation, and mixing are essential for engine mixture preparation. Additional challenges arise in NH_3 reforming prior to combustion due to the need to mix liquid ammonia with gaseous hydrogen, aside from the distinct low boiling point of ammonia. To address this, novel NH_3-H_2 injection approaches will be developed, including H_2-saturated NH_3 injection and internal/external NH_3-H_2-mixing injection. This will be based on a hierarchical ensemble of experimental (Kneer/Reddemann) and numerical (Schröder & Pitsch) investigations, covering studies on single droplets, droplet stream, nozzle internal mixing and degassing, as well as jets and sprays in high-pressure chambers. Additionally, injection strategies using aero-spike ejectors for liquefied ammonia will be explored to utilize the compression and liquefaction work stored in liquid ammonia to enhance mixing and potentially replace turbochargers or intercoolers (Schmitz).

To assess and optimize the novel approaches at engine level, experimental investigations will be conducted on both thermodynamic and optical single-cylinder engines (Pischinger). The former will focus on efficiency and emission characteristics, while the latter will provide optical access for additional insights into ammonia combustion, such as ignition sites and flame propagation. Special emphasis will be placed on developing catalytically controlled and temperature-controlled pre-chamber ignition to eliminate the need for a spark plug, resulting in smaller pre-chamber volumes and reduced efficiency losses. This will be complemented by numerical simulations to deepen the understanding of combustion concepts, including mixture inhomogeneities, temperature distributions, pollutant formation, and efficiency losses.

Mechler/ Eichel

4.5.2.2 Ammonia fuel cells

Add short summary here.

Conventional fuel cells run on pure H_2 as a fuel on the anode. In a global H_2 economy, this H_2 can originate from NH_3 as a transport vector, releasing H_2 in a decomposition process. However, for the use in state-of-the-art low-temperature fuel cells, ultra-pure H_2 is needed. Thus, after an NH_3 reformation process further purification steps might be needed to remove traces of NH_3 and other catalyst poisons, or more poison tolerant materials would need to be developed. On the other hand, it is also possible to use NH_3 directly. In such direct ammonia fuel cells (DAFC), NH_3 is either converted catalytically or, in the case of solid oxide fuel cells (SOFCs), internally reformed to N_2 and H_2 due to the high temperatures used. This direct conversion has the potential for higher overall efficiencies, as the intermediate step of NH_3 reformation is omitted and, in case of SOFCs, the heat from the exotherm fuel cell reaction can also be utilized by the endotherm ammonia decomposition. Within the fuel science center, we aim to investigate both low- and high-temperature fuel cells and develop suitable catalysts, fuel cell designs and operation strategies. Besides aiming for improved performances and economic viability, we will consider effects of cross-over, poisoning and the relevance of NO_x formation.

Previous work

The concept of direct ammonia fuel cells (DAFCs) have been proposed already about 50 years ago for both low-temperature [REF] as well as high temperature applications [163]. While the latter originally aimed to produce NO by direct oxidation of NH3, it was also found that by tuning the catalyst composition, ammonia can be completely decomposed into H_2 and N_2 at the high operating temperatures above $700°C$ [163, 159, 157, 155]. Nevertheless, in conventional solid oxide fuel cells (SOFC) utilizing oxide conducting ceramics like yttrium-stabilized zirconia (YSZ), NH_3 can directly react with the O^{2-} transported causing NO_x formation [163]. Alternatively, solid proton conducting fuel cells (SPCFC) 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 [148, 129, 126], this also causes new challenges, for instance in developing the right catalyst to decompose ammonia at those lower temperatures [157, 175]. Typical materials for SPCFC electrolytes are yttrium-doped barium zirconate ($BaZrO_3$, BZY), cerate ($BaCeO_3$, BCY) or zirconate-cerate ($Ba(Ce, Zr)O_3$, BCZY). The cerium contributes to a high proton conductivity, however, BCY is chemically instable. The zirconate on the other hand is more stable, but the sinterability and conduction is low [148, 130]. The zirconate-cerate combines high conductivity with increased stability. Further doping with Yb improves the stability even more [129, 126, 138]. Typical fuel electrodes for the development of hydrogen fuel cells are composites (cermets) of yttrium-doped barium cerates or zirconates and nickel (Ni). As Ni shows high NH_3 decomposition activity, these materials have also

been investigated for direct ammonia fuel cells [?]. Importantly, the catalyst and ion conducting ceramic also need to be stable towards both NH_3 as well as $NH_3/H_2/N_2$ mixtures.

PI Eichel contributes extensive experience in the field of material and cell development for SOFCs, both in fuel cell and electrolysis mode [108, 104, 113, 111, 112]. They have developed a novel SPCFC with promising results at 600 °*C* [109]. Also a first analysis of the potential use of those systems with NH3 as a fuel has been recently explored [105]. Further competences are contributed by PI Pischinger in the operation of fuel cell test benches [86] as well as fuel cell simulation, including system performance, locally resolved electrochemical behavior within a cell, and mechanical stress distribution within the different cell materials [51, 48, 70]. At the TME, furthermore, a single-cell SOFC test rig is currently being set up and first dedicated SOFC simulation models were developed to investigate fuel cell and reformer performance with different gaseous fuels.

On the low-temperature side first achievements have been demonstrated in literature, but there the use of noble-metal catalysts, accompanied by the risk of catalyst poisoning, is a critical factor. Furthermore, membranes that are long-term stable in the NH3-environment still need to be optimized. Efforts to improve DAFC efficiency focus on finding new catalysts for ammonia oxidation (AOR) and oxygen reduction reactions (ORR), as well as suitable anion exchange membranes (AEM) [172, 115, 137, 117, 131]. Recent works have shown promising results obtained from a low-temperature DAFC, achieving power densities exceeding 100 mW/cm2 (up to 420 mW/cm2) from a single cell. These studies typically utilize platinum-based catalysts [116, 171, 133, 178, 142]. However, the high cost and susceptibility of platinum to poisoning with AOR intermediates have led to research combining it with other materials (e.g., Pt-Ir, Pt-Ir-Ni, Pt-CeO2, Pt/C) [151, 123, 167, 140, 154, 145] or exploring non-noble alternatives, like nickel-based catalysts (e.g., Ni, Ni-Cu, Ni-Cu-Fe, Ni-Cu-Co, Ni-Ag) [179, 144, 174, 176, 173, 162, 118]. Unfortunately, for the Ni-based materials the AOR onset potential is high (close to the oxygen evolution reaction – OER), which might lead to formation of oxygenated nitrogen species (i.e., nitrogen oxides, nitrates, nitrites) as undesirable byproducts [179, 118, 146]. Different solutions are proposed to overcome this problem, such as decoration of the Ni-based materials with Pt or Ag nanoparticles [162, 161], use of a conducting support (e.g., carbon materials) [174, 176, 173] or modification with oxyanions [132].

The group of PI Mechler has long-standing experience in the characterization and development of fuel cells and non- or low-noble metal catalysts.[18, 85, 78, 53] Furthermore, in preliminary studies Ni- and Ni-Cu-hydroxides as catalyst materials were investigated as catalysts for AOR. We found that the Ni-Cu hydroxides possess better catalytic activity than pure NiOH2 for AOR (Fig. 4.8a). Additionally, supporting them on reduced graphene oxide (rGO) and carbon nanotubes (CNT) as conductive supports further increased their performance (Fig. 4.8b).

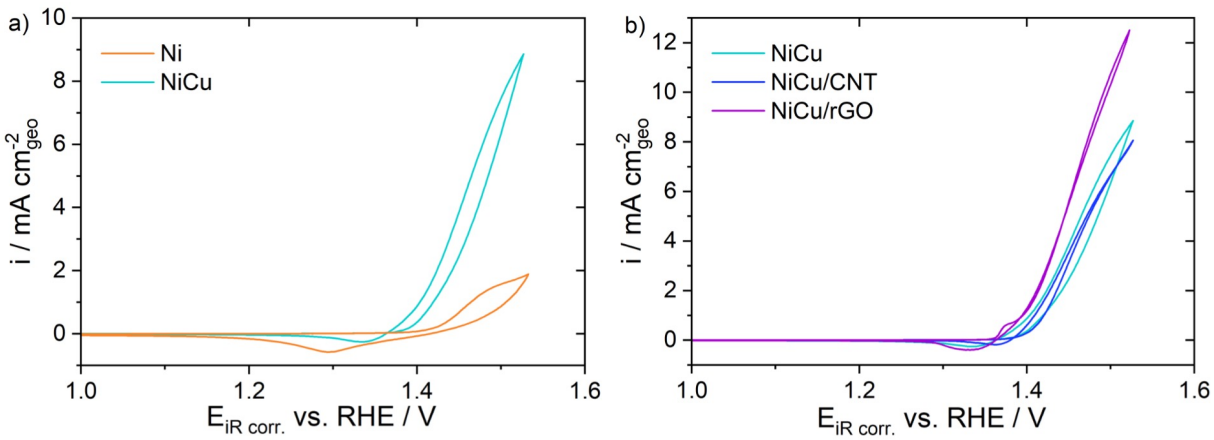

Figure 4.8: Rotating disc electrode measurements in 1 M KOH + 0.5 M NH_4OH for a) pure Ni- and Ni-Cu-hydroxides; b) Ni-Cu-hydroxides supported on CNTs and rGO.

The use of a potentially liquid fuel in comparison to gaseous hydrogen furthermore requires the rethinking of the fuel cell design, for instance electrolyte distribution and cell design. The group of PI Schröder has experience in the simulative and experimental evaluation of various flows, including both single phase as well as mixed liquid-gas-phases in electrochemical environments.[26, 12, 84, 83, 31] This can be utilized to optimize flow geometries for different forms of NH3-supply, i.e. as liquid NH3, gaseous NH3 or dissolved NH3.

Eventually to add input from LCA-side.

Eventually to add membranes from Wessling (see carbon-based fuel cells)

Objectives

We aim to improve systems that can directly convert NH_3 electrochemically in direct-ammonia fuel cells (DAFCs). The materials used at low-temperature are easily deactivated by NH_3, so we will develop new, poison resistant electrode and alkaline membrane materials. At high temperatures we want to focus on solid proton conductors to prevent any risk of NOx formation. In order to improve NH_3 decomposition at the lower operating temperatures, we also work on improved catalyst materials. Integration into single cells is necessary to evaluate the performance and impact of operation conditions. Also reaction and degradation mechanisms of all components need to be considered. To obtain these objectives, the following goals are defined:

- Development of new AOR catalysts, poison resistant cathodes and advanced proton conductors & alkaline membranes
- Understanding reaction & degradation mechanisms in single cell operation
- Characterize and mitigate the impact of NOx formation

- Compare the efficiency with NH_3-H_2-PEMFC pathway

Furthermore, links between NH_3 activation for chemical synthesis with respect to the full conversion in a fuel cell will be investigated (ref. Ch. XXX). The economic viability of the direct ammonia conversion and the possible integration into a hydrogen economy are highly relevant (ref. Ch. XXX).

Work program

For the characterization of state-of-the-art as well as newly developed SOFCs and SPCFCs the test bench at the TME (PI Pischinger) will be commissioned. Here, extensive test sequences are planned to optimize the operation strategies upon characterization of side product formation (e.g., NOx) as well as degradation. Also the impact of feed stream compositions and blends will be characterized. The tests will further be supported by multi-scale simulation on the system level. At the lab of PI Eichel, the proton conductors studied in previous work will be further developed towards reduced thickness of the electrolyte while ensuring that the electronic leakage is low. Furthermore, new materials will be developed to enhance the NH_3 decomposition at the lower operating temperatures. For NH_3 decomposition Ni-based catalysts show promising performances. However, the long-term stability especially in NH_3 atmosphere has not been studied in detail and thus is the next step. Thus, the NH_3 fuel cell is investigated in long-term tests of at least 500 h with accompanied current-voltage characteristic and impedance spectroscopic measurements to understand the degradation mechanisms.
For the characterization of low-temperature fuel cells, also a test-station will be constructed and operated. Meanwhile, catalytic studies are conducted ex-situ, for instance in rotating disc electrode environment as well as half-cell configurations with gas-diffusion electrodes. New materials will be developed based on previous experience, for instance based on single-atom catalysts, as well as in collaboration with PI Palkovits based on their synthesis platforms and predictions of novel catalysts by PI Khetan. Design-of-experiment will be conducted in collaboration with PI Mitsos to optimize the reaction conditions in the fuel cell. For the construction of the full cells, the contributions by PI Schröder will be utilized. In this project, micro-PIV experiments are envisioned for volumetric flow field measurements of narrow channels and channel structures, experimental analysis of the interaction of gas bubbles and fluid flow in narrow channels, and the investigation of rough surface structures in narrow channels. The measurements will be complemented by numerical simulations using the m-AIA simulation framework. This work will be utilized for an optimized design of fuel distribution in flow channels, optimized flow rates and eventually electrode designs that facilitate mass transport. The fuel cell topic will be embedded in studies of economic viability and the possibility for integration into a future hydrogen economy. Contributions from PI v.d. Aßen as well as PI Mitsos will evaluate

[XXX] (see chapter XXX).

4.5.2.3 N-emission control

Khetan

For an efficient aftertreatment of the complex mixture of exhaust gases (NO_x+N_2O) and reducing NH_3 slip, developing an innovative NH_3 combustion system is the first essential step [160, 168]. One potential strategy is catalytic combustion, which offers advantages over conventional non-catalytic combustion, including reduced NO_x emissions due to lower operating temperatures and high efficiency. To successfully use this strategy, advanced in-cylinder coating materials need to be synthesized that promote NH_3 combustion reaction to reduce N_2O and NO_x emissions, catalytically as well as through minimized wall heat loss. Another innovative idea is to use residual heat and unburnt NH_3 for in situ H_2 generation[124], which can then be used to assist exhaust after treatment via H_2-SCR [120]. The inhibitory effect of O_2, NO_x, and H_2O on N_2O decomposition in the exhaust stream remains poorly understood [136, 152, 143]. Current N_2O decomposition catalysts are comprised mainly of precious metals that require high operation temperatures [177, 153, 147]. Catalysts with no or low-precious metal content need to be developed that are functional at lower temperatures, capable of handling exhaust composition variations, resistant to sulfur poisoning, and have high solvothermal stability. 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. This can be achieved by spectroscopic operando monitoring of reaction intermediates on the catalyst surface and accelerated reactive molecular dynamics simulations. Unconventional methods like microwave (MW) activation [158] show promise in enhancing reaction rates but have yet to be employed in NH_3-combustion exhaust stream purification. These approaches can break inherent scaling relations based on the Sabatier principle [156], which fundamentally limits the maximum activity of any conventional catalyst. A non-equilibrium MW-driven approach to deoxygenate an oxide catalyst material may enable the splitting of N_2O. To achieve this, promising materials and the corresponding aftertreatment test benches need to be identified that can work well under MW irradiation.

Previous work

The FSC has already successfully demonstrated the potential of alternative fuels both in pure form and in mixtures in conjunction with innovative combustion and aftertreatment concepts for reducing pollutant emissions such as CO, NOx, and unburned hydrocarbons [72, 3, 80, 101, 63]. To achieve high combustion efficiency with highly diluted fuel/air mixtures in combustion engines, we recently performed the deposition and characterization of perovskite ($La_{0.8}Sr_{0.2}CoO_3$: LSCO) catalyst for in-cylinder engine coating [101]. As shown in Fig. 4.9, with this strategy, the effective flame quenching distance was reduced

and the catalytically active coating led to reduced hydrocarbon and carbon monoxide emissions. Furthermore, we have demonstrated successful microstructural and surface defect engineering of several oxide materials, for which an enhancement of catalytic activity towards both the CH_4- and CO-oxidation was shown [ClusterRefToBeAdded]. Besides innovative coatings and material design, we have made several gainful strides in 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 [63, 37, 49, 17] [106]. 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 [37, 49, 17] [106]. However, these catalysts are mostly inactive for N2O decomposition at such low temperatures. Our investigations [3, 80] as well as other's [125, 119] indicate that the efficient decomposition of N_2O is facilitated above 450 $°C$, and in industrial applications, only above 700 $°C$. This necessitates the development of new catalysts that allow for coupled deNOx-SCR and N_2O decomposition under technologically relevant conditions.

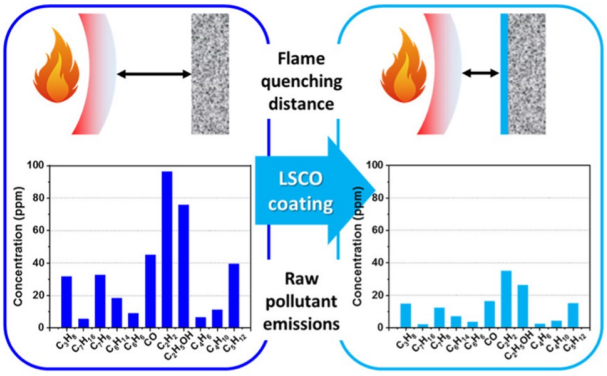

Figure 4.9: Schematic showing the catalytic activity enhancing effect of in-cylinder coated LSCO from our preliminary work.[101]

We have previously identified universal descriptors of catalytic activity in doped oxides [?] and rationalized the effect of strong-metal-support interactions [107, 110]. Recently, we employed the first principles-based energetic span model (ESM) to analyze N2O decomposition activity on precious metal (Ru, Rh), and hybrid (Ru/Cu, Rh/Cu, Ru/Ni, Rh/Ni) catalysts.[ClusterRefToBeAdded] Our work reveals excellent opportunities for enhancing N2O decomposition by exploiting weak correlations between intermediates' adsorption free energies. We reported the first Brønsted-Evans-Polanyi relation for N_2O decomposition, which enabled mechanistic analysis of various binding energies on the turnover frequency (TOF), as shown in Fig. 4.10. The ESM captures the inhibitory effects of surface-adsorbed NO on N_2O decomposition. The strong binding energy of adsorbed N_2 and O adatom is found to aid the catalytic activity in the presence of NO (Fig. 4.10b) but becomes limiting in its absence (Fig. 4.10a). While this simple model is very informative, 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

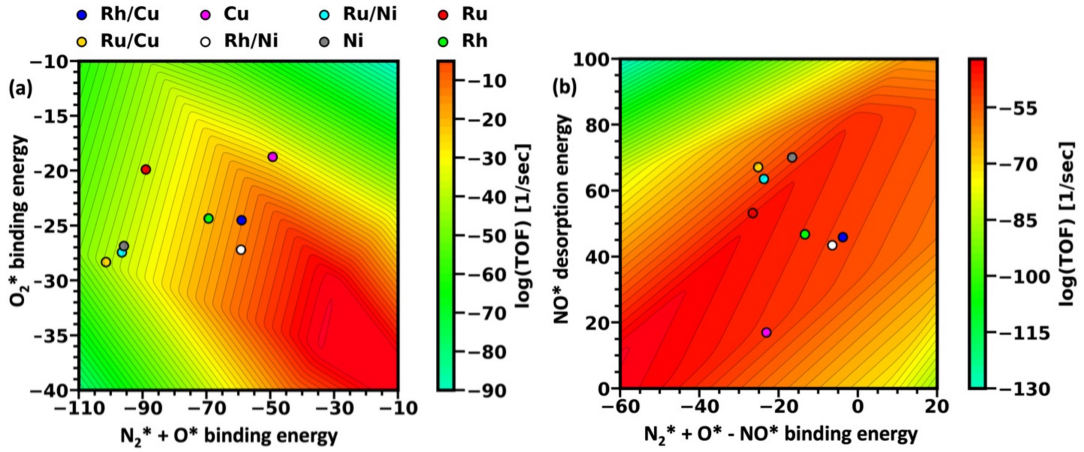

Figure 4.10: TOF activity maps from our previous work [ClusterRefToBeAdded] showing the predicted performance of various catalysts (a) in the absence of NO, and (b) in its presence. The inhibitory presence of NO reverses the catalyst ordering and leads to a significant overall drop in TOF.

cold-start phase, we recently introduced an MW-assisted heterogeneous catalytical setup [66]. 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.

Objectives

The overall goal of this sub-project is to develop Exhaust After-treatment Systems (EATS) for NH3 combustion comprising of no or low precious metal catalysts that are functional at lower temperatures, capable of handling wide variations in exhaust composition, resistant to sulfur poisoning, and have high solvothermal stability. Our objectives are:

1. Implementation of new approaches to reduce N_2O and NO_x emissions at the combustion stage using in-cylinder catalysis and in-situ catalytically generated H_2.

2. Design and characterization of new catalysts for coupled N_2O decomposition and NO_x reduction in conventional as well as MW-stimulated EATS.

3. Development of spectroscopic setups for exhaust gas component analysis and reactive molecular dynamics simulations for operando modeling of reaction intermediates.

Work program

To achieve the first objective, we will build upon our preliminary work [101] to perform in-house synthesis of advanced cylinder catalytic coating materials that promote more effi-

cient NH_3 combustion thereby reducing N_2O and NO_x emissions. We will focus especially on oxide and the relatively unexplored nitride catalysts to engage their surface available O and N vacancies, respectively, as active sites. The catalyst design will also account for their thermal insulation properties, such that the heat loss through the walls can minimized to achieve higher combustion efficiency. As an innovative step forward, we will also explore the use of residual heat and unburnt NH_3 for in situ H_2 generation [124], which can then be used to assist exhaust after treatment via H_2-SCR [120]. To achieve this, we will perform the synthesis and characterization of oxide-supported transition metal catalysts. The synthesis route, including reactor design and process conditions, will be tailored to the microstructural and compositional requirements for the targeted catalyst material and may involve surface engineering on the particle level,

To achieve coupled DeNOx-SCR with unburnt NH_3 and N_2O decomposition, we will develop transition metal-promoted zeolite catalysts, such as in our recently shown direct methane partial oxidation [24]. 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 stoichiometry and emission. The target will be to use MW irradiation to generate oxygen or nitrogen defects in oxides or nitrides, respectively, and thereby enable the splitting of N_2O. Furthermore, we will develop new strategies to enable cyclic heated zones to achieve a constant N_2O decomposition. At the material scale, we will identify promising catalysts that can work well under MW irradiation. We will also explore the possibility of MW-driven NH_3 dehydration to produce H_2 in situ, which can then be used to assist with H_2-SCR. These efforts will be complemented by non-equilibrium molecular dynamics simulations under the effect of finite electric fields [169, 165], which will help estimate the dielectric losses and surface reactivities of potential MW-susceptible materials. The simulations will also consider dopant and vacancy effects on the dielectric loss factors, which will ultimately influence the reactivity. After validating these simulations against experimental data, we will connect material properties to material function by using non-parametric techniques such as symbolic regression or compressed sensing [164]. These efforts can yield easily calculable descriptors of dielectric loss for material screening without resorting to expensive large-scale simulations.

We will complement our device and material development efforts with spectroscopic operando monitoring of reaction intermediates and products at the catalysts' surface using In-situ DRIFTS, impedance, and mass spectrometry. We will perform accurate mass-spectrometric quantification of the NH_3 combustion exhaust and NO_x/N_2O 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 energetic span model [127, 128], and analyze the catalyst's stability vs. activity. Going beyond 0 K first-principles calculations, we will simulate the operando interfacial structures and reactive events during aftertreatment using reactive and machine learning interatomic potentials [134, 166]. 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.

4.5.3 Strategic Research Area – Concatenated Synthetic Pathways

PIs: Palkovits (coordinator); 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

The challenges at the molecular level for the transformation of renewable resources and energies are usually addressed individually by the respective catalysis disciplines of molecular and heterogeneous catalysis, electro-, or biocatalysis for specific reaction steps along the value chain. The focus lies on the activation of hydrogen, ammonia, carbon dioxide, and biomass using tailor-made catalysts for selective cleavage and formation of chemical bonds to increase molecular complexity. 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, targeting the integration of catalytic transformations and potentially even unit operations on the levels of catalyst, reactor and process. Therein, the individual 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. 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 Strategic Research Area (SRA).

Scientific basis forms already at an early development stage the important link between the transformation steps with a focus on the transfer points of intermediate products, reaction media, and the recycling of the catalyst system. Therefore, the selection of the most appropriate catalytic discipline is not determined by evaluation of the individual catalytic transformation, but rather by the most efficient contribution within a transformation cascade of concatenated catalytic steps. On the catalyst level, concatenated transformation sequences can be achieved by combining several catalysts from one or various catalytic disciplines or by enabling several transformations within one catalyst, e.g., by installing more than one type of active site. On the reaction level, catalytic transformation cascades in one solvent system as well as multiphase reactions are targeted. On the reactor level, compartmentalization, throughout customizing of interphases and tailored process intensification by means of multiphase reaction systems combined with reactive separation present important objective.

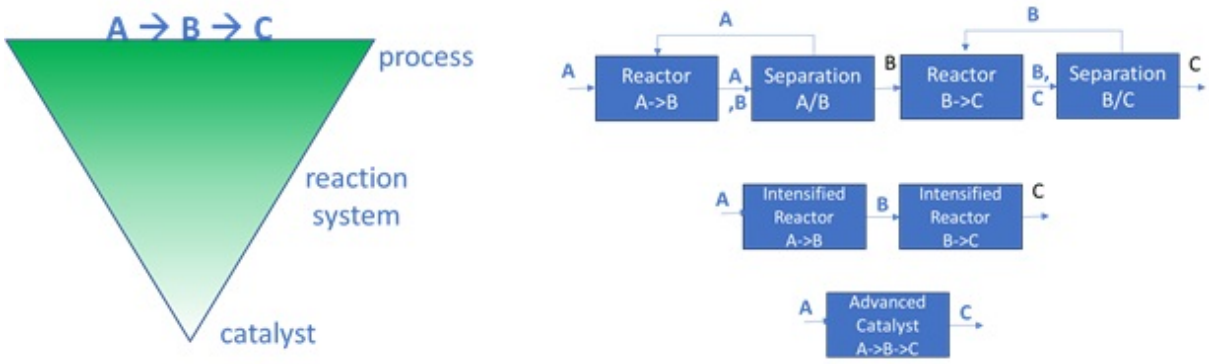

Figure 4.11: ?

Strategy and Structure of SRA

Concatenated synthetic pathways are considered on different length scales. At the molecular level, the focus is on catalysts for bio-hybrid syntheses that allow accessing the same products from different carbon resources and via different catalytic pathways or that provide chemical compounds structurally composed of motifs from different carbon sources. Within the reaction cascade, interconnected catalytic systems aim at an optimum combination of catalytic transformations along a value path towards maximum resource efficiency at minimum energy needs and operational costs (unit operations). Ultimately, several catalytic transformations are combined – potentially even combined with reactive separation – in integrated reactor systems.

Objectives:

- Catalyst systems integrating more than one functionality either within one catalyst type or by combining a multitude of catalysts to enable transformation sequences
- Mono- and multiphasic reaction systems enabling transformation sequences catalysed by different catalysts
- Optimum transformation sequences enabled by compartmentalization, tailored interphases and process intensification

Klankermayer

4.5.3.1 Bio-hybrid synthesis

Add short summary here.

On the one hand, bio-hybrid syntheses spans methodologies of accessing the same products from different carbon resources and via different catalytic pathways. On the other hand,

it provides chemical compounds structurally composed of motifs from different carbon sources. Examples of the former comprehend alcohols and acids as well as their derivates which can be derived from CO_2 or biomass transformations with either chemo-, bio-, or electrocatalysis. The latter relates to e.g. linear and cyclic acetals as well as alkyl carbonates accessible by the combination of biogenic alcohols and CO_2.

Previous work

Objectives

Work program

Rother 4.5.3.2 Interconnected catalytic systems

Add short summary here.

Old: In order to leverage the greatest potential to achieve novel, sustainable, effective processes for hybrid fuels or chemicals, the aim of interconnected catalytic systems is 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 can be combined. These advantages include not only effective synthesis to high product concentrations with high purity and low waste streams, but also the lowest possible energy input and high eco-efficiency. 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 are available for modular, flexible combinations. The outstanding element of this approach in The Fuel Science Center (FSC) is the techno-economic overall balancing of the process, including reprocessing (if necessary), in order to be able to make honest statements.
In addition, the adaptive use of sustainably obtained starting materials from biomass or various CO_2 capture methods is a complementary element of the interconnected catalytic systems.

Interconnected catalytic systems aim at an optimum combination of catalytic transformations along a value path towards maximum resource efficiency at minimum energy needs and operational costs (unit operations). An example comprehends the biocatalytic alcohol synthesis followed by homogeneously catalysed acetal production within the same solvent system.

Previous work

Objectives

Work program

Jupke 4.5.3.3 Integrated reactor systems

Add short summary here.

On the device level, concatenated catalytic systems require the potential integration of several catalytic transformations as well as unit operations within integrated reactor systems. Multiphase reaction systems interlinking two sequential catalytic transformations in different phase present an example of the approach.

Previous work

Objectives

Work program

4.5.4 Strategic Research Area – Translational Catalytic Processes

PIs: Leitner (coordinator); 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 (4.5.X), 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 X, 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 CO2-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 X, right). The translation of chemical pathways to processes covers the entire technology maturity progression, from laboratory experiments with model substances to interlinked unit operations comprising upstream feedstock supply, catalytic transformations, downstream processing, and product isolation. 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.

Figure 4.12: ?

Strategy and Structure of SRA

The research in the Strategic Research Area (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.

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.

Blank

4.5.4.1 Feedstock complexity and variability

Add short summary here.

Previous work

Objectives

Work program

4.5.4.2 Feedstock supply and integrated Conversion

Palkovits

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/complex feedstocks in a potentially variable or even adaptive manner. Additionally, for feedstocks such as CO_2 an integrated supply, separation, and conversion can be envisaged.

Previous work

Within the diverse feedstock base, carbon dioxide poses specific challenges. It is either provided by direct air capture (DAC) associated with high energy demands, in form of carbonate or amine solutions from scrubbing processes or as (highly) diluted and multi-compound feedstock stream directly from air or other chemical processes.
Environmental merit order curves were developed to rank CO_2 sources according to their environmental impact over the available CO_2 supply to identify favourable locations for CO_2 utilization with lowest environmental impacts, so-called CO_2 oases (Van der Aßen).[91, 59][x] More system level?
Efficiency of carbon capture is inevitably determined by the utilized absorbent or adsorbent as well as process design. Especially tailored adsorbents bear the potential to significantly reduce the energy demand of DAC. Nitrogen containing carbons present a promising material class allowing to tailor capacity and selectivity, respectively. Major design parameters comprehend material morphology including porosity, pore sizes and specific surface for overall capacity as well as surface functionality determining basicity and hydrophilicity where the latter plays a major role in the competitive adsorption of CO_2 and water.

- Previous work Palkovits on N-containing carbons in CO_2 adsorption[88, 87, 89]
- Previous work Eichel on N-containing carbons[77, 57]

Integrated capture and conversion processes present a promising alternative to the sequential CO_2 capture, storage and release of CO_2 followed by its conversion. As a first step, coupling of CO_2 capture by amine wash with subsequent CO_2 reduction were demonstrated:

- Previous work Leitner, Jupke[76, 2, 25], Blank[36], Palkovits[46]

Beyond CO_2, also the selective separation of biomass-based intermediates such as sugars, carboxylic acids, amino acids and diols[73, 23] 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

Objectives

Work program

Leitner 4.5.4.3 Energy and feedstock fluctuation and variability

Add short summary here.

Previous work

Objectives

Work program

4.5.5 Strategic Research Area – Resilient & Adaptive Conversion Systems

PIs: von der Aßen, Walther (coordinators); Arning, Leicht-Scholten, Mitsos. ARs: Backhaus, Venghaus, Ziefle.

Add short summary of SRA here

We develop an integrated approach for the design and operation of fuel and 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 individual processes and process paths to the broader supply chain and system level.

At the level of fuel and chemical conversion systems we incorporate the objectives of resilience and sustainability to process design and electrochemical systems. At value chain level, we develop an integrated approach merging descriptive and prescriptive system and policy analysis with ex-ante risk assessment and policy design to enable the prescriptive design of resilient and sustainable global fuel and energy conversion value chains. We use Life-cycle assessment for multiple scales, from devices (in production and in fuel conversion), over production processes to the supply chains.

2 Sentences LCA & Systems Engineering

Strategy and Structure of SRA

Overarching objectives

- Unify definition of resiliency across scales and formalize this mathematically
- Unify definition of adaptivity across scales and formalize this mathematically

We expand the scope to a global system's perspective. The complex cross-sectorial and cross-industrial interdependencies between energy, mobility and chemistry are captured, regarding also for conversion paths, chemical energy carriers, and fuels that are not explicitly captured in the other subprojects of FSC^2 (e.g., integrating maritime and aviation transport, xxx). This serves as a prerequisite for the modelling of system-wide transformation processes with explicit mapping and evaluation of competition and synergies between potential technologies, energy carriers, transport trajectories, fuels, and chemicals. The design of a resilient and adaptive conversion system for sustainable energy carriers and chemicals is achieved based on systemic risk measures, stakeholder-specific decision-models, social perceptions and requirements, prospective policy design and dynamic transformation processes.

Mitsos #### 4.5.5.1 Process design and operation

We develop optimization-based methods for the design and operation of resilient and adaptive sustainable production processes.

Previous work

- Best of a kind algorithms for robust nonlinear programs Djelassi, H., Mitsos, A. Global Solution of Semi-infinite Programs with Existence Constraints. J Optim Theory Appl 188, 863–881; 10.1007/s10957-021-01813-2 (2021).
- Optimization tools Zingler, A., Jungen, D., Djelassi, H. , Mitsos, A. libDIPS — Discretization-Based Semi-Infinite and Bilevel Programming Solvers. Optimization Online. (2023) `https://optimization-online.org/?p=24914`, accessed 10.01.2024
- Flexibility in process engineering Schäfer, P., Schweidtmann, A. M., Mitsos, A. Nonlinear scheduling with time-variable electricity prices using sensitivity-based truncations of wavelet transforms. AIChE Journal 66; 10.1002/aic.16986 (2020).
- Optimization with machine learning programs embedded Schweidtmann, A. M.; Bongartz, D., Grothe, D., Kerkenhoff, T., Lin, X., Najman, J., Mitsos, A. Deterministic global optimization with Gaussian processes embedded. Math. Prog. Comp. 13, 553–581; (2021).

Objectives

The objectives are as follows:

- Overcome the limit of current production processes which exhibit insufficient flexibility to cope with volatility of renewable energy and feedstocks and in economic boundary condistions.
- Incorporate the objectives of flexibilty, resilience, and adaptivity into the process design
- Utilize surrogate modelling, based on machine learning concepts, to overcome computational expense
- Integrate two-stage stochastic and robust approaches to model uncertainty

Work program

- Mitsos: Combined stochastic and robust approaches for adaptive & resilient processes

- Pitsch: High-fidelity multiphysics numerical simulations and model development for multiphase flows in electrochemical systems

4.5.5.2 System integration

Walther

We develop an integrated approach merging system and policy analyses with ex-ante systemic risk assessment and stakeholder-specific decision models to design resilient, adaptive, and sustainable global value chains for energy carries and chemicals. We apply data mining, machine learning and text analysis for policy and system analysis, qualitative and quantitative social and risk sciences methods for risk assessment, agent-based simulation and bilevel optimization for modelling of stakeholders' decisions, and robust/stochastic multi-objective optimization and complex-dynamic simulation for the design of resilient and sustainable value chains.

Previous work

The target of Competence Area 3 (CA3) in FSC was to develop a system-wide design perspective to guide and evaluate novel transformation pathways over all involved scales for the transformation towards flexible conversion systems for bio-hybrid fuels. The 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.

The framework accounts for the sector-coupling between the electricity and fuel production with descriptive and predictive system's analysis and prescriptive system's design.

Currently, technical, environmental, economic, and social challenges still prevent the market adoption and diffusion of renewable fuels. Thus, barriers to market adoption and diffusion were analyzed in FSC applying a holistic analytical approach combining micro-level (DEMATEL improved by K-means) and macro-level (ISM modeling improved with MMDM) analysis ([27]). Results confirmed economic and technical supply chain challenges (costs - B1, technologies - B4, infrastructure - B5) as important barriers, but also the role or lacking public perception (acceptance - B2, awareness

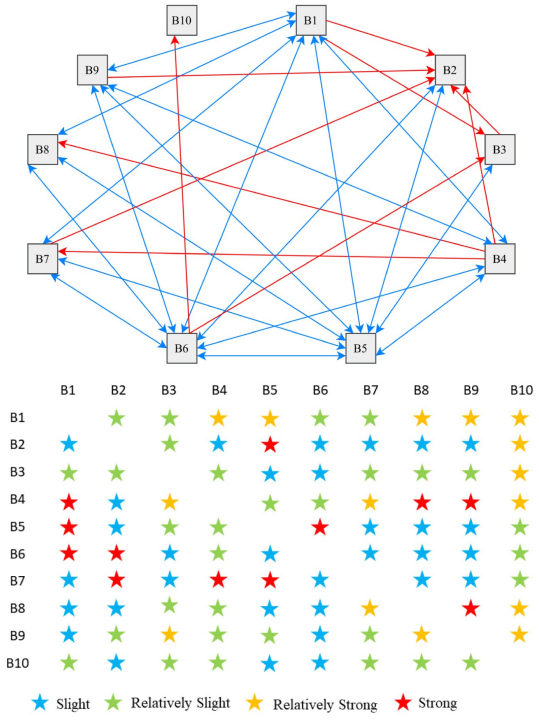

Figure 4.13: Cause and effect relationships between the market development barriers (top) and im-

- B3), insufficient regulation and policies (B6), missing stakeholder coordination (B7), lacking feedstock availability (B8), and environmental challenges (B9). This re-emphasizes that all of these aspects have to be tackled to allow for the planning and design of renewable fuel conversion systems and corresponding supply chains.

Figure

To account for economic and technical supply chain barriers, all supply chain stages (resource availability, technologies, import, demand) and their interlinkages were analyzed in detail. On the input side, we showed how short- and long-term availability of feedstocks determine technology choice and structure of supply chains ([99, 28, 95]AmiriZenodo24). In strong cooperation with Competence Area 1 (CA1) and Competence Area 2 (CA2), innovative technologies and process paths were evaluated regarding not only techno-economic, but also environmental criteria (Alexander, Niklas, ggf. Quellen wiederholen). On the output side, (meta-)analyses provided information on the future demand of fuels for different scenarios ([9]). To determine prospective fuel candidates, different fuels were compared against market diffusion barriers and sustainability factors based on a possibility-based multi-criteria approach ([27, 90]Hendiani24). In FSC^2, such analyses will gain even more importance with the current discussion on the role of energy carriers as transport vectors, storage options, fuels and potential platform chemicals, and requires an even stronger focus on the analysis and design of integrated fuel and chemical conversion systems.

Figure

To account for the high importance of public perception on the market diffusion of sustainable fuels and innovative fuel production technologies, research in FSC analyzed the multi-faceted perspective of risks and benefits in more detail. A new, multi-stage iterative empirical methodology was developed combining initial qualitative assessments (interviews, focus groups, media analysis) and quantitatively evaluations (ANOVAs, regressions, cluster analyses, structural equation modeling). This research revealed risk perception of fuels as a complex construct, segmented into distinct domains such as health, environment, and technical risks (Figure xx), influenced by cognitive and affective components [4] and individual factors [81]. Research showed that perception of sustainable technologies can strongly improve by communication of benefits (e.g., for e-fuels and CCU technology infrastructure), but that there is also the thread of misconceptions, especially for innovative technologies with little prior knowledge in the lay public (e.g., CCU) [54], which could lead to oversimplified heuristics or misconceptions, erode trust, and effects openness [75, 62, 79, 38]. To allow for better informed decisions, a new distance-to-ideal-solution approach was developed to integrate expert opinions (policy makers, investors,

R&D) on environmental, social, and economic aspects of renewable energy systems [?]. Based on these works, advanced risk assessment methods will be developed in FSC^2 accounting for systemic risks of global supply chains instead of segmented and isolated technology-related risks, integrating expert knowledge and stakeholder-specific risk perception profiles. Also, an integrated risk communication framework is needed to ensure consider and integrate public demands, comprehensibility, align public and expert views, build trust, and support informed decisions [82].

To account for the strong influence of policy and regulatory frameworks, the implementation of fuel-related policies in various policy sectors (e.g., energy, transport, fuel, agriculture, fiscal, and environmental policy) as well as on different scales (global, European, national, but also regional) requires transparency and coherence [65, 58, 29] Therefore, 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 no or negligible explicit inclusion was found in other relevant policy fields like biomass utilization, bio-economy, water, or environmental policies [90](Torkayesh1d, Torkayesh1e,). Also, the techno-economic and social perspectives are only insufficiently considered under current policy design compared to the environmental perspective (Torkayesh1d). 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.

FigureFigureMoving beyond these descriptive and predictive analyses, the above-mentioned aspects were integrated to design optimal fuel and energy systems developing prescriptive optimization models. Planning models account for long-term transformation, variability in feedstock availability, import scenarios, and high integration of the fuel and energy sector. A MILP supply chain design model was developed using a cyclic time decomposition approach to capture long-term planning horizons for the transformation towards climate-neutrality as well as short-term variability of feedstocks ([99]). Sector-integration was regarded in an energy system optimization model investigating interdependencies between synthetic fuel production and required investments and dispatch in infrastructures for electricity, hydrogen, methane, and liquid fuels [10, 11, 95, 35]. For these complex models, myopic approaches proved appropriate by reducing the computation time drastically, while still providing adequate objective values [95]. 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 [94]. Based on these techno-economic optimization approaches, an extended model explored the trade-offs between cost, land-use, and water-use via a multi-objective model solved by the augmented epsilon constraint method. Results for

an European Union (EU) case study implied that a comprehensive increasing in costs of 10% could reduce land- and water-use significantly [28]. First approaches also integrated policy requirements into energy and fuel conversion system planning as a prerequisite for future endogenous policy design [102, 41]Zardoshti;. Moreover, an innovative approach was developed integrating cost and social acceptance in the optimization-based design of bio-hybrid fuel supply chains [6, 50]. To account for limited resource availability in Europe and expected importance of fuel imports [27, 94], potential global energy trade scenarios were analyzed using a bi-objective optimization model balancing cost with inequality. The latter is measured by the Gini-coefficient as per capita economic value added by energy production. Findings reveal that inequality could be halved with a slight cost increase of 10% [45]. 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. Also, the various uncertainties until the target year 2050, such as European policies, final energy demand, water availability, and potential areas for renewable energy sources that so far were mainly regarded by exogenous scenarios must be regarded endogenously when designing resilient conversion systems for energy carriers and chemicals. Additionally, specific stakeholder perspectives (investors, political decision makers, operators, customers) and the interlinkage between system level design and stakeholders' behavior must be considered explicitly.

Objectives

An integrated approach is developed for the design and operation of resilient and adaptive conversion systems for energy carriers and chemicals merging system design and systemic risk assessment with stakeholder and policy analysis to achieve resilient system design. The approach is innovative as it enhances existing approaches by:

i) extending the system boundary to account the multi-sectorial effects between 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 with endogenous modelling of import options and transport vectors,

ii) establishing a systemic risk assessment framework by quantifying and evaluating the impact and interrelations of a wide range of endogenous and exogeneous transformative and operational risks. This includes the incorporation of systemic risk perception to better understand and address the subjective factors affecting risk assessment and management.

iii) developing an agent-based approach that is explicitly regarding stakeholders' perspectives and their influence on the overall system's level and vice versa,

iv) 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.
Overall, 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.
Figure: fuel and energy conversion system beeinflusst durch Risks - Stakeholders – Policy Resilient System Design als Transforamtion

Work program

multi-sectoral and global model

Energy carriers and platform chemicals play pivotal roles in the transformation of the relevant sectors energy, mobility, and chemistry. An integrated perspective on the transformation processes of these sectors is therefore imperative. To overcome the limitations of sectoral models, a prescriptive LP/MILP optimization model is developed accounting for all the sectors and stages and technical, environmental, and (socio)economic aspects. This needs strong cooperation of researchers from engineering, business administration, and socioeconomic analysis (Mitsos, van der Aßen, Walther, Venghaus). This model is fed with data from artificial intelligence (AI)-supported system analysis of regional, national, European, and global transformation strategies and roadmaps with a cross-sectoral perspective covering all process-paths and stakeholders in the value chains of energy, mobility, and chemistry as well as all potential resources, intermediate and (by-)products, and import vectors. Challenges result from the broad system boundary and integrating the hierarchy's device – process (path) – supply chain in sufficient accuracy. Modeling can be based on first proof-of-concept cross-sectorial chemistry-energy model (Niklas - ...,), bioeconomy[52] and fuel-energy import models (Grit - Afrika/ORIES Paper). This cross-sectorial, hierarchical model lays the foundation for integrating systemic risk measures, stakeholder perspectives and policy design (see below), and the conclusive model for the design resilient and adaptive fuel and chemical conversion systems.
Figure: Devices – Prozesspfade – Supply Chains – System
Ex-ante systemic risk measurement and communication approach
Employing energy carriers as storage mediums and transport vectors has significant impor-

tance for balancing the globally unevenly distributed and fluctuating supply and demand. However, this goes along with considerable (geo-)political, technical, economic, environmental, natural, and social risks (e.g., [5]). Thus, FSC^2 replaces the so far often isolated assessment of risks and risk perceptions of single technologies or fuels by a more complex systemic risk landscape. These risks are then integrated into a stakeholder-specific (politics, investors, public) risk communicated framework to enable preventive mitigation of risks, especially during the transformation stage of the fuel and chemical conversion systems (Walther, Venghaus, Arning, Ziefle).

Assessment of systemic risks (Walther, supported by Venghaus) targets at identifying and prioritizing risks, and determining interrelations between risks. Besides classical qualitative (expert opinions, subjective judgements) and quantitative (probabilistic likelihood and impact models) methods, advanced AI-based methods are used, e.g., machine learning (ML) for pattern recognition, predictive modeling, and identification of correlations and dependencies between different sectors, energy carriers and countries, or natural language processing to extract insights from unstructured data sources (news articles, regulatory documents, social media, national, and industrial roadmaps). As a result, estimates of risk levels are available to support decision-making processes, and uncertainties can be quantified as input for modeling the design of resilient and adaptive fuel and chemical conversion systems. Perception of systemic risks (Arning, Ziefle) is determined based on social and risk sciences merging qualitative (interviews/focus groups analysed either by grounded theory or Mayrings's content analysis approach) and quantitative methods (surveys which assess risk perception, sociodemographic data, and attitudinal constructs). 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 are derived. Advanced inferential statistical methods (regression analyses, MANOVAs) combined with structural equation modelling are utilized to identify and understand factors and their interrelations. As a result, systemic risk perceptions and their impact across different sectors (local impact of broad-scale decisions) are available.

A risk communication framework (Arning, supported by Venghaus, Walther & Ziefle) is developed in FSC^2 based on the risk perception and risk assessment results. This framework will be tailored to address the complex and systemic nature of risks and considers individual factors such as dual-route information processing, varying levels of trust and expertise in a increasingly complex media and information context. It enhances dialogue through careful message and communication process design, adhering to principles of trust and transparency. The framework integrates technical details with broader systemic risk contexts with the aim to offer stakeholders a balanced perspective for informed decision-making in a systemic risk context.

Interrelations Stakeholder – System

Stakeholders' (consumers, investors, policymakers) targets, perceptions and decision-making significantly impact the market and technology diffusion [34, 44, 42, 40]Arning/Venghaus. However, models often still follow a centralized perspective (e.g., [16, 20, 64, 28, 99, 95]. Thus, FSC will integrate behavioral aspects of stakeholders into scale-up and transformation strategies and policy design (Walther, Venghaus, supported by Arning).

Stakeholders' role and position in the value chain, objectives, constraints, perceptions, and risks are analyzed using (social) network analysis, data mining, ML, and social empirical research. This allows to derive stakeholder-specific decision models. Mapping these within an agent-based simulation model, the behavior and interrelations between stakeholders can be analyzed. To analyze the interrelation between overall system's development and stakeholder decisions, a bilevel optimization approach is used with the upper level representing the development of the overall fuel and chemical conversion system, and the lower level representing stakeholders such as utility companies or investors with their specific business models. Analyzing the underlying non-cooperative relationship allows to determine the most influencing factors for stakeholders' and overall system's development as well as trade-offs, synergies and contradictions between the two levels, promising (legal) incentives and policies.

Ex-ante Policy Analysis and Design

A coherent and efficient policy framework is imperative for resilient conversion systems. FSC will develop a policy assessment framework with a cross-sectoral policy assessment dashboard, incorporating reverse policy assessment and ex-ante national and European policy design considering global and geopolitical developments (Venghaus, supported by Walther).

A policy monitoring dashboard is developed covering systematic policy monitoring 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. Quantitative approaches like decomposition analysis, econometric analysis, data mining & ML as well as qualitative techniques including climate policy integration, text analysis, natural language processing, and multi-criteria coherence analysis are applied. Policy coherence is optimized for various potential policy scenarios, and optimal policies are designed using mathematical and optimization models. Innovative reverse policy assessment is carried out determining 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.

Resilient Value Chain Design

Resilient and adaptable value chains are needed to cope with multiple economic, technical, environmental, geopolitical, legal, natural, and social stressors ([27]1a, more Literature). So far, uncertainties are mostly regarded applying scenario or sensitivity analysis,

or stochastic or robust optimization ([40, 43]Literatur). However, often only individual uncertainties and risks are accounted for, and interrelations between uncertainties, or relations between uncertainties, (systemic) risks and resilience criteria are mostly neglected. Thus, an integrated approach for the design of resilient fuel and chemical value chains is developed. First, relevant resilience criteria for fuel and chemical value chains (e.g., redundancy, diversity, optionality, multi-functionality, flexibility, loose coupling, adaptivity) are derived merging knowledge from different disciplines like ecology, engineering, control theory, supply chain management, or energy systems analysis. Criteria are then classified and characterized, and dynamic cause-and-effect relations between uncertainties, risks, and resilience are derived regarding intended and unintended effects, short- and long-term effects, feedback loops, or delays among system components. The developed System Dynamics model allows insights in how the system behavior evolves in response to disturbances or changes and provides a qualitative understanding of resilience dynamics facilitating scenario exploration, complexity management, and participatory decision-making (Literatur). The results of these analysis are then aggregated and fed into a prescriptive optimization model for the design of resilient conversion systems for energy carriers and chemicals. In this model, resilience criteria, risks, and uncertainties can either be integrated into the objective, or as a constraint, as a probability or a (worst-case) scenario. 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 transport-vectors, diversified resources, enhanced facility fortifications, or (short- and long-term) energy storage.

Overall resilience model

Results are integrated in the Resilience Design Appraoch regarding for resilience criteria for value chains such as redundancy, diversity, multifunctionality (Literatur) as well as resilience criteria of technologies and process paths like adaptability and flexibility (Alexander), and fulfilling sustainability criteria from Life Cycle Assessment (Niklas). (Walther). Trade-offs, contradictories and similarities between resilient, economic, and sustainable solutions can be determined.

4.5.5.3 Life-cycle assessment

v. d. Aßen

Add short summary here. We use LCA for multiple scales, from devices (in production and in fuel conversion), over production processes to the supply chains.

Previous work

Objectives

Work program

- von der Aßen: Flexible Green Chemicals: Enhancing the Resilience of Fuel, Energy, and Chemical Supply
- von der Aßen: Prospective absolute environmental sustainability assessment of sector-coupled transitioning fuel supply chains
- Backhaus: Improved methods for comparative foot- and handprints: facilitating the development of least-toxic and sustainable fuels
- Greiff: tbd

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

[1] Method for the Experimental Determination of the Bunsen Absorption Coefficient of Hydraulic Fluids, volume ASME/BATH 2019 Symposium on Fluid Power and Motion Control of Fluid Power Systems Technology, 10 2019.

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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 4 pages for this section.

5 Structures and strategies in the Cluster of Excellence

5.1 Support of early-career researchers

Table 5.1: Funding Request for Early-career Support

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
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 4 pages for this section.

5.2 Support of equity and diversity

Table 5.2: Funding Request for the Support of Equity and Diversity

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
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

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) content-driven 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 co-operations. 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

Forschungsdatenmanagement

Research Data Management
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 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 [98] (see Table 5.3), 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 [8][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 The Fuel Science Center (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 5.1). 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.

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.

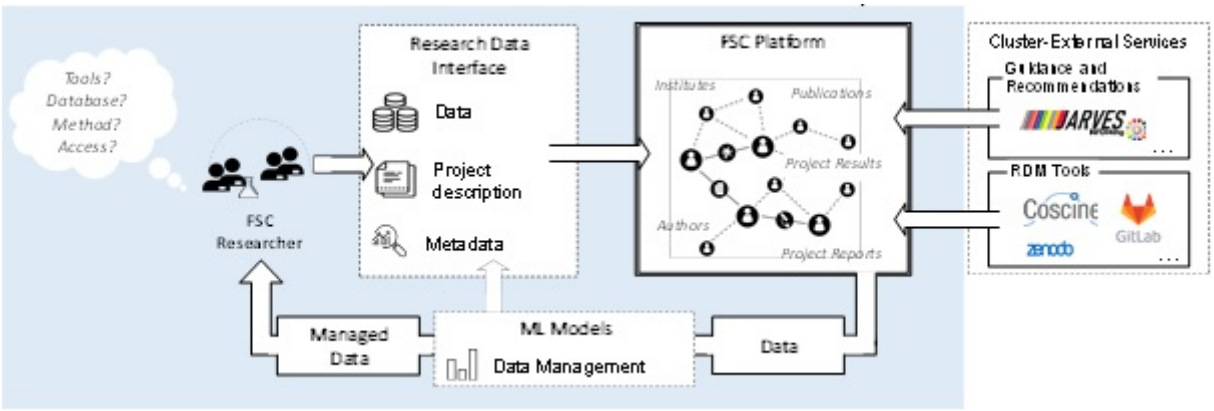

Figure 5.1: RDM concept within the cluster's platform.

Table 5.3: 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 5.4: Funding Request for Research Data Management, Infrastructures and Instrumentation

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
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 4 pages for this section.

5.4 Management, governance, quality assurance

Quality assurance

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

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
Staff							
Direct project costs (excluding staff)							
Instrumentation							

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

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 4 pages for this section.

5.5 Science communication, knowledge transfer and research-oriented teaching

Intra-cluster communication

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 (Competence Areas (CAs), Translational Research Teams (TRTs), general assembly, situational working groups). Intensification and documentation of intra-cluster communications will be supported by RWTH Aachen University (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 5.6: Funding Request for Science Communication, Knowledge Transfer, and Teaching

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
Staff							
Direct project costs (excluding staff)							
Instrumentation							

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 3 pages for this section.

6 Environment of the Cluster of Excellence

6.1 Strategic development planning at the applicant university/universities

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 3 pages for this section.

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 3 pages for this section.

6.3 Collaboration with external partners

Table 6.1: Funding Request for Collaboration with external partners

	2026	2027	2028	2029	2030	2031	2032
Funding category	Totals per year in euros, rounded to the nearest thousand						
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 Programme

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 euros, rounded to the nearest thousand

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 euros, rounded to the nearest thousand

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							
Doctoral researchers							
Other staff							

Table 7.4: Total Funding Requested

	2026	2027	2028	2029	2030	2031	2032	Total 2026-2032
Funding category	Totals in euros, rounded to the nearest thousand							
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.1: Total Expenditure by category

	2019	2020	2021	2022	2023
	Totals per year in euros, rounded to the nearest thousand				
Staff					
Professors					
Junior research group leaders					
Postdocs					
Doctoral researchers					
Other research staff					
Direct project costs (excl. research staff)					
Instrumentation > €100,000					
Total expenditure					

Table A.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.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 euros, rounded to the nearest thousand

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

A.5.2 Effects of the Coronavirus Pandemic

Table A.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: Staff diversity – gender

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