

The Integrated Fuel & Chemical Science Center

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

Contents

1 General data						
2	2 Summary of the proposal					
3	Juster of Excellence	9				
4	Res	earch F	Program		15	
	4.1	Resear	ch objecti	ves, research approach, and positioning within the research area	15	
	4.2	Prelim	inary and	previous work	17	
	4.3	Structu	are of the 1	research program	19	
	4.4	Staff a	nd institut	ional composition of the Cluster of Excellence	21	
	4.5	Detaile	ed descript	tion of the research program	23	
		4.5.1	Resilient	& adaptive conversion systems	23	
			4.5.1.1	Value chains	23	
			4.5.1.2	Life-Cycle Assessment	23	
			4.5.1.3	Systems engineering	23	
		4.5.2	Translati	onal catalytic processes	23	
			4.5.2.1	Feedstock complexity and variability	24	
			4.5.2.2	Carbon capture and conversion	24	
			4.5.2.3	Adaptive catalytic systems	24	
		4.5.3	Concater	nated synthetic pathways	24	
			4.5.3.1	Bio-hybrid synthesis	24	
			4.5.3.2	Interconnected catalytic systems	24	
			4.5.3.3	Integrated reactor systems	24	
		4.5.4	Ammoni	a conversion	24	
			4.5.4.1	Ammonia combustion	24	
			4.5.4.2	Ammonia fuel cells	24	
			4.5.4.3	N-emission control	24	
		4.5.5	Carbon-l	based fuel conversion	24	
			4.5.5.1	Backwards compatible fuels	24	
			4.5.5.2	Adaptive engine concepts	24	
			4.5.5.3	Organic fuel cells	24	
	4.6	Supple	ementary i	nformation on legal and ethical aspects of the research program	26	

5	Stru	ictures	and strategies in the Cluster of Excellence	29
	5.1	Suppor	rt of early-career researchers	29
	5.2	Suppo	rt of equity and diversity	31
	5.3	Strateg	gies for research data and research software management and provisions	
		for res	earch infrastructures and instrumentation	44
	5.4	Manag	gement, governance, quality assurance	46
	5.5	Scienc	e communication, knowledge transfer and research-oriented teaching	48
6	Env	ironme	nt of the Cluster of Excellence	51
	6.1	Strateg	gic development planning at the applicant university/universities	51
	6.2	Resour	rces provided by the institution(s)	53
	6.3	Collab	oration with external partners	55
7	Fun	ding R	equest	57
Α	Арр	endix		59
	A.1	The 25	5 most important publications for the Cluster of Excellence, Category A .	59
	A.2	The 25	5 most important publications for the Cluster of Excellence, Category B .	61
	A.3	The 25	5 most important additional qualification indicators	63
	A.4	Propos	al for a university allowance	65
		A.4.1	Overall concept of the applicant university/universities regarding strate-	
			gic orientation and the university allowance	65
		A.4.2	Envisaged use of the university allowance	65
	A.5	Data o	n the first funding period	67
		A.5.1	Data on the first funding period	67
		A.5.2	Effects of the Coronavirus Pandemic	67

Guidlines 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. DrIng. (USA) Stefan Pischinger

Further spokesperson(s)	Institution			
Prof Dr. vor. not Walter Leitner	RWTH Aachen University			
FIOL DI. IEI. nat. Walter Leither	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/Institu	Field of expertise	Position
1	JunProf. Dr. phil. Katrin Arning	Aachen, RWTH	Risk Perception and Communication	W1/temporary [LB1]
2	Prof. DrIng. DiplWirt.Ing. Niklas von der Aßen	Aachen, RWTH	Technical Thermodynamics	W3/permanent
3	UnivProf. DrIng. Lars M. Blank	Aachen, RWTH	Applied Microbiology	W3/permanent
4	Prof. Dr. rer. nat. habil.	Jülich, FZJ	Fundamental Electrochemistry	W3/permanent
4	Rüdiger Eichel	Aachen, RWTH	Material and Process of Electrochemi- cal Energy Storage and Conversion	w 5/permanent
5	UnivProf. Dr. Kathrin Greiff	Aachen, RWTH	Anthropogenic Material Cycles	W3/permanent [LB2]
6	UnivProf. Dr. rer. nat. Sonja Herres-Pawlis	Aachen, RWTH	Chair of Bioinorganic Chemistry	W3/permanent
7	Prof. DrIng. Karl Alexander Heufer	Aachen, RWTH	Chair of High Pressure Gas Dynamics	W3/permanent
8	UnivProf. DrIng. Andreas Jupke	Aachen, RWTH	Chair of Fluid Process Engineering	W3/permanent
9	UnivProf. Dr. rer. nat. Jürgen Klankermayer	Aachen, RWTH	Institute of Technical and Macromolec- ular Chemistry (Translational Molecu- lar Catalysis)	W3/permanent
10	UnivProf. Dr. rer. nat. habil. Lars Lauterbach	Aachen, RWTH	Synthetic Microbiology Teaching and Research Area	W2/permanent
11	UnivProf. Dr. rer. nat. Walter Leitner	Aachen, RWTH	Institute of Technical and Macromolec- ular 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	UnivProf. Dr. rer. nat. Anna Mechler	Aachen, RWTH	Chair of Electrochemical Reaction En- gineering	W3/temporary
14	UnivProf.	Aachen, RWTH	Chair of Process Systems Engineering	W3/permanent
<u> </u>	Alexander Mitsos, Ph.D.	Jülich, FZJ	Energy Systems Engineering	() S/permanent
15	UnivProf. Dr. rer. nat. Regina Palkovits	Aachen, RWTH	Institute of Technical and Macromolec- ular Chemistry (Heterogeneous Cataly- sis and Technical Chemistry)	W3/permanent
16	UnivProf. DrIng. (USA) Stefan Pischinger	Aachen, RWTH	Chair of Thermodynamics of Mobile Energy Conversion Systems	W3/permanent
17	UnivProf. DrIng. Heinz Pitsch	Aachen, RWTH	Institute for Combustion Technology	W3/permanent
18	UnivProf. Dr. rer. nat. Dörte Rother	Jülich, FZJ	Institute of Bio- and Geosciences	W3/permanent
19	UnivProf. Dr. Franziska Schoenebeck	Aachen, RWTH	Chair of Organic Chemistry I and Insti- tute of Organic Chemistry	W3/permanent
20	UnivProf. Dr. phil. Carmen Leicht-Scholten	Aachen, RWTH	Chair of Gender and Diversity in Engi- neering	W3/permanent

No.	Principal investigators	Location/Institu	Field of expertise	Position
21	UnivProf. Dr. rer. nat. Ulrich Simon	Aachen, RWTH	Chair of Inorganic Chemistry and Elec- trochemistry	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	UnivProf. DrIng. Matthias Wessling	Aachen, RWTH	Chair of Chemical Process Engineering	W3/permanent
25	UnivProf. 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 Tech-	Saudi Arabia
0	nology	Saudi Alabia
9	Massachusetts Institute of Technology	USA
10	Utrecht University	The Netherlands

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

Guidlines 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

Crude oil fuels 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. The *de-carbonization* of the energy sector imposes challenges and opportunity for the *de-fossilization* of the sectors mobility and chemistry where direct electrification is difficult or even impossible. Shaping the development of the post-fossil future requires novel research concepts as basis for disruptive technologies resulting in major societal and economic changes. "The Fuel Science Center (FSC)" 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.

Guidlines 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

Crude oil fuels 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 greenhouse gas 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 [?], p. 29. The scenarios for the reduction towards net zero require a range of measures centered around the global availability of renewable energy. The resulting *de-carbonization* of the energy sector imposes challenges and opportunity for the *de-fossilization* of the sectors mobility/transportation and chemistry where direct electrification is difficult or due to the indispensable need for carbon even impossible. [REF] Shaping a postfossil era at the interface of energy and chemistry therefore requires novel research concepts as basis for disruptive technologies that will result in major societal and economic changes.

In the context of this dynamic development of utmost importance for a sustainable future, "FSC" 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 and its strategic partners FZJ and 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.

Mission

FSC has its roots in the Cluster of Excellence "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 in on-road propulsion systems and the molecular structure and composition 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. In the subsequent phase, FSC was able to establish the broader field of "fuel science" internationally by overcoming disciplinary borders through composing the extended competencies of the network according to the time- and length-scale of the molecular, device, and systems level. Translational research teams were formed to foster collaboration and scientific exchange on specific research questions. While carbon-based fuels where 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 CO₂ as alternative carbon sources could



Figure 3.1: Vision of FSC 2.0 "The Fuel 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".

thus be envisaged. Expanding the research topics beyond the technosphere demonstrated the importance of adaptivity as important design criteria to cope with the dynamics and variations in energy and feedstock supply at the interface between the energetic and chemical sectors.

The successfully established concept of interdisciplinary Competence Areas (CAs) and their effective and dynamic interconnection now form the backbone of the fully integrated research framework in the next phase of FSC. All research activities and projects are fully allocated within Strategic Research Areass (SRAs)? where they absorb and vice versa stimulate the disciplinary progress of the individual Principal Investigators (PIs), thus constantly augmenting the CAs. This structure has been devised to allow for adaptive response to the global developments at the interfaces of the energy, mobility, and chemistry sectors on basis of scientific and methodological excellence. With the specific infrastructure of the partner institutions and the scientific profiles of the involved PIs, FSC is ideally positioned to align the 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 thermal as well as electrical 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.

10

Objectives

The SRAs for FSC will address the following key questions originating from the vision and mission outlined above:

- 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?
- How can engines and devices be designed to exploit ammonia as fuel most effectively?
- 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?
- How can chemical, biochemical, and electrochemical transformations for the manipulation of C-O and C-N bonds be interlinked to open **concatenated synthetic pathways** to fuels and chemicals?



• Systems approach?

Figure 3.2: Strategic Research Areass (SRAs).

The SRAs are bridged via general design challenges that will be addressed in flexible working groups as the research progress develops. This includes for example the integration of production pathways and propulsion properties for the C-based fuel design, the fundamental mechanisms of electrochemical ammonia activation for energy or synthetic applications, the seemingly contradicting goals of integration for process chains and flexibility of individual

CHAPTER 3. OBJECTIVES OF THE CLUSTER OF EXCELLENCE

process steps, and **...???** The central platform for the discussion, analysis, and continuous adjustment of the overall research program in light of its mission and vision is provided in the "Systems Design Forum (SDF)".



Figure 3.3: Systems Design Forum (SDF).

Scientific approach

CAs as the backbone Short: Specific strengths of FSC, next major methodological developments,... Research Program SRAs descriptions => REIHENFOLGE FESTLEGEN! The Systems Design Forum Working groups; role and workflow of the forum

Guidlines 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

Guidlines 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

Guidlines for section 4.3:

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

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

Content: Point out CAs as success.

4.3 Structure of the research program

Guidlines for section 4.4:

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

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

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

4.4 Staff and institutional composition of the Cluster of Excellence

Guidlines 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.

Estimation: 13 pages per subsection.

4.5 Detailed description of the research program

4.5.1 Resilient & adaptive conversion systems

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

4.5.1.1 Value chains

Add short summary here.

Previous work

Objectives

Work program

4.5.1.2 Life-Cycle Assessment

4.5.1.3 Systems engineering

Table 4.1: Proposed Staff in Research Subunit x

	2026	2027	2028	2029	2030	2031	2032
Staff category			Num	ber of pe	rsons		
Professors							
Independent junior research group lead-							
ers							
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 Translational catalytic processes

PIs: Leitner (coordinator); von der Aßen, Blank, Jupke, Klankermayer, Mayrhofer, Mitsos, Palkovits, Pitsch, Rother, Simon, Waldvogel, Wessling, Zobel. ARs: Khetan, Leonhard, Mag-

nus, Wiegand.

4.5.2.1 Feedstock complexity and variability

4.5.2.2 Carbon capture and conversion

4.5.2.3 Adaptive catalytic systems

4.5.3 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.

4.5.3.1 Bio-hybrid synthesis

4.5.3.2 Interconnected catalytic systems

4.5.3.3 Integrated reactor systems

4.5.4 Ammonia conversion

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

4.5.4.1 Ammonia combustion

4.5.4.2 Ammonia fuel cells

4.5.4.3 N-emission control

4.5.5 Carbon-based fuel conversion

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

4.5.5.1 Backwards compatible fuels

4.5.5.2 Adaptive engine concepts

4.5.5.3 Organic fuel cells

Guidlines 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.

CHAPTER 4. RESEARCH PROGRAM

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

Guidlines 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									

Guidlines 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

rSC 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 childcare 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) contentdriven team interactions within the Competence Areas and the Translational Research Teams, (ii) individual mentoring through senior and junior research group leaders, (iii) regular self-teaching activities as well as (iv) exposure and shaping of networks with outside partners and stakeholders in the form of company visits, international conference participation, and visiting periods at internationally renowned universities (Universities of California, Tsinghua, Melbourne University, and universities of our cooperation partners). FSC encourages their Ph.D. students to also supervise smaller projects together with B.Sc. and M.Sc. students in order to develop leadership skills. Scientific cooperation and team work will further knit a strong network between the early career researchers. A strong scientific mentoring by two supervisors, where applicable from different disciplines, will be mandatory.

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

Junior Research Group Leaders: These outstanding researchers have received their Ph.D. degree, excelled during a postdoctoral position and develop towards independent project leaders. They are encouraged and supported through the Advanced Talents Program to acquire their own budget through prestigious grants (Emmy Noether, ERC Starting Grant, Helmholtz junior research group etc.) and other research projects, supported by a mentor within the FSC or the RWTH program. To foster excellence at this career level, it is important to provide time and freedom for their research, an attractive scientific environment and intellectually stimulating 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 \in 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

Guidlines 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

Table 5.3: 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								

Guidlines 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.

CHAPTER 5. STRUCTURES AND STRATEGIES IN THE CLUSTER OF EXCELLENCE

5.4 Management, governance, quality assurance

81	0	/		•			
	2026	2027	2028	2029	2030	2031	2032
Funding category	Total	s per yea	r in euros	, rounded	to the ne	arest thou	isand
Staff							
Direct project costs (excluding staff)							
Instrumentation							

Table 5.4: Funding Request for Management, Governance, Quality assurance

Guidlines 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

Table 5.5: 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								

Guidlines 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

Guidlines 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)

Guidlines 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							

Guidlines 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: 7	Fotal Funding	Requested for	the Research	Programme
---------------------	----------------------	----------------------	--------------	-----------

Research Subunits	Funding category	Total* 2026-2032
	Staff	
Subunit A	Direct project costs	
	(excluding staff)	
	Instrumentation	
	Staff	
Subunit B	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 in-	
strumentation	
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	r of staff j	oositions		
Professors							
Independent junior research group lead-							
ers							
Postdoctoral researchers							
Doctoral researchers							
Other staff							

	2026	2027	2028	2029	2030	2031	2032	Total 2026- 2032
Funding category		Total	s in euros	, rounded	l to the ne	arest tho	usand	
Staff								
Direct project costs (excl.								
staff)								
Instrumentation								
Total project funding								

Table 7.4: Total Funding Requested

Guidlines 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.

Guidlines 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 58 hich, 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.

A Appendix

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

Guidlines 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

Guidlines 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

Guidlines 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.

Guidlines 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.

Guidlines 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

Guidlines for A.5.1:

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

Guidlines 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 eur	os, rounded t	o 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
		Nu	mber of pers	ons	
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 in-	
strumentation	
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 par- ticipating 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						