Letter of Intent to submit a proposal for a Cluster of Excellence

1. Proposal Type

☐ New proposal
Reference number of draft proposal: **EXC 3_____/0**

☒ Renewal proposal
Reference number of establishment proposal: **EXC 2186/1**

2. 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

3. Applicant university/universities and spokesperson(s)

Managing University
RWTH Aachen University

Spokesperson(s)

Authorised spokesperson at 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

4. Participating Institutions

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

5. 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 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.

In the context of this dynamic development of utmost importance for a sustainable future, **The Integrated Fuel & Chemical Science Center (FSC²) generates fundamental knowledge and novel scientific methods for the development of adaptive technical solutions to valorize renewable electricity and feedstocks into liquid energy carriers and chemicals in a systems approach**. 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.

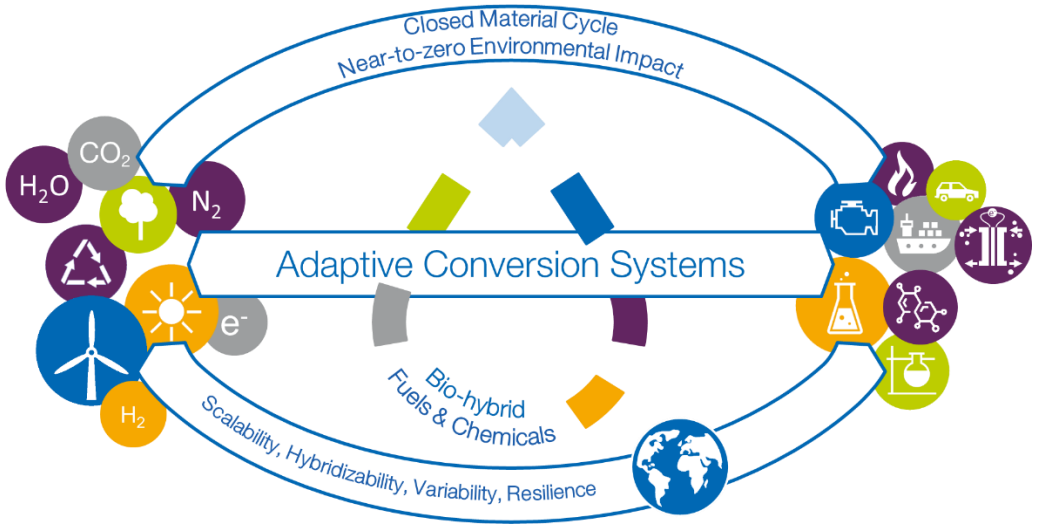

Figure 1: Vision of FSC² „The Integrated Fuel & Chemical Science Center generates fundamental knowledge and novel scientific methods for the development of adaptive technical solutions to valorize renewable electricity and feedstocks into liquid energy carriers and chemicals in a systems approach”

FSC² has its roots in the 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 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 Competence Areas (CAs) and their effective and dynamic interconnection now form the backbone of the **unique research framework of The Integrated Fuel & Chemical Science Center (FSC²) 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 PIs, thus constantly augmenting the CAs. With the specific infrastructure of the partner institutions and the scientific profiles of the involved PIs, FSC² 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**.

The Strategic Research Areas for FSC² will address the following key questions originating from the vision and mission outlined above:

⇨ *How can global energy and material cycles be made **adaptive and resilient**, while fulfilling all three dimensions of sustainability - **ecological, economic and social**?* Current research often focuses on individual aspects of fuel and chemical conversion systems, e.g., individual levels of the system, or certain aspects of sustainability. Moreover, disruptions to the systems' supply and operation are often neglected, and the dynamics of the ongoing long-term transformation towards climate-neutrality are not sufficiently covered. Therefore, there's 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 pathways** to fuels and chemicals?* The transformations of bio-based, C1 and N1 building blocks are usually addressed by the individual catalysis disciplines of molecular, heterogeneous, electro- or 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.

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 electrochemical ammonia activation for energy or synthetic applications, as well as the seemingly contradicting goals of integration for process chains and flexibility of individual process steps. 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**, where the progress of the five SRAs and the working groups is biannually reported and discussed.

Figure 2: The integrated framework of the five Strategic Research Areas (SRAs) embedded within the Competence Areas (CAs)

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.

6. Principal Investigators

No.	Principal investigators	Location/Institution	Field of expertise	Position
1	**Jun.-Prof. Dr. phil. Katrin Arning**	**Aachen, RWTH**	**Risk Perception and Communication**	**W1/ tenure track**
2	**Prof. Dr.-Ing. Dipl.-Wirt.Ing. Niklas von der Aßen**	**Aachen, RWTH**	**Technical Thermodynamics**	**W3/permanent**
3	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
		RWTH	Material and Process of Electrochemical Energy Storage and Conversion	
5	**Prof. Dr. rer. nat. Kathrin Greiff**	**Aachen, RWTH**	**Anthropogenic Material Cycles**	**W3/permanent**
6	**Prof. Dr. rer. nat. Sonja Herres-Pawlis**	**Aachen, RWTH**	**Bioinorganic Chemistry**	**W3/permanent**
7	Prof. Dr.-Ing. Karl Alexander Heufer	Aachen, RWTH	High Pressure Gas Dynamics	W3/permanent
8	Prof. Dr.-Ing. Andreas Jupke	Aachen, RWTH	Fluid Process Engineering	W3/permanent
		Jülich, FZJ	Integrated Bio-Refineries	
9	Prof. Dr. rer. nat. Jürgen Klankermayer	Aachen, RWTH	Translational Molecular Catalysis	W3/permanent
10	**Prof. Dr. rer. nat. habil. Lars Lauterbach**	**Aachen, RWTH**	**Synthetic Microbiology**	**W2/permanent**
11	**Prof. Dr. phil. Carmen Leicht-Scholten**	**Aachen, RWTH**	**Gender and Diversity in Engineering**	**W2/permanent**
12	Prof. Dr. rer. nat. Walter Leitner	Aachen, RWTH	Technical Chemistry and Petrochemistry	W3/permanent
		Mühlheim a.d.R., MPI CEC	Molecular Catalysis	
13	Prof. Dr. techn. Karl Mayrhofer	Erlangen, FZJ	Electrocatalysis	W3/permanent
14	**Prof. Dr. rer. nat. Anna Mechler**	**Aachen, RWTH**	**Electrochemical Reaction Engineering**	**W2/temporary**
15	Prof. Alexander Mitsos, Ph.D.	Aachen, RWTH	Process Systems Engineering	W3/permanent
		Jülich, FZJ	Energy Systems Engineering	
16	Prof. Dr. rer. nat. Regina Palkovits	Aachen, RWTH	Heterogeneous Catalysis and Technical Chemistry	W3/permanent
		Jülich, FZJ	Sustainable Hydrogen Economy	

No.	Principal investigators	Location/Institution	Field of expertise	Position
17	Prof. Dr.-Ing. (USA) Stefan Pischinger	Aachen, RWTH	Thermodynamics of Mobile Energy Conversion Systems	W3/permanent
18	Prof. Dr.-Ing. Heinz Pitsch	Aachen, RWTH	Combustion Technology	W3/permanent
19	Prof. Dr. rer. nat. Dörte Rother	Jülich, FZJ Aachen, RWTH	Synthetic Enzyme Cascades	W2/permanent
20	Prof. Dr. rer. nat. Franziska Schoenebeck	Aachen, RWTH	Organic Chemistry	W3/permanent
21	Prof. Dr. rer. nat. Ulrich Simon	Aachen, RWTH	Inorganic Chemistry and Electrochemistry	W3/permanent
22	**Prof. Dr. rer. nat. Siegfried R. Waldvogel**	**Mühlheim a.d.R., MPI CEC**	**Electrosynthesis**	**W3/permanent**
23	Univ. Prof. Dr. rer. pol. Grit Walther	Aachen, RWTH	Operations Management	W3/permanent
24	Prof. Dr.-Ing. Matthias Wessling	Aachen, RWTH	Chemical Process Engineering	W3/permanent
25	**Prof. Dr. rer. nat. Mirijam Zobel**	**Aachen, RWTH**	**Crystallography and X-Ray Spectroscopy**	**W3/permanent**

7. Fields of Research

No.	Fields of research
1	403-02 Technical Chemistry
2	404-01 Energy Process Engineering
3	404-02 Technical Thermodynamics
4	403-01 Chemical and Thermal Process Engineering
5	404-04 Hydraulic and Turbo Engines and Piston Engines
6	321-01 Inorganic Molecular Chemistry – Synthesis and Characterisation
7	321-02 Organic Molecular Chemistry – Synthesis and Characterisation
8	204-01 Metabolism, Biochemistry and Genetics of Microorganisms
9	112-03 Business Administration
10	111-02 Empirical Social Research

8. Key Methods and Models

No.	Method / Model
1	Chemical Synthesis and Molecular Systems
2	Multifunctional Catalyst Design
3	Electrochemistry and Electrocatalysis
4	Metabolic and Bioprocess Engineering
5	Multi-Scale Reactor Design
6	Fluid Dynamics and Reactive Flows
7	Process Systems Engineering
8	Combustion Science and Engineering
9	Exhaust Gas Aftertreatment Systems
10	Sustainability and Risk Assessment

9. Collaborations/Conflicts of Interest

No.	Collaboration partners	Location/Institution
1	Claire Adjiman	United Kingdom; Imperial College London
2	Paul Alivasatos	USA; University of California
3	Frédéric Allain	Switzerland; ETH Zürich
4	Paul Anastas	USA; Yale University
5	Jakob Andreasson	Czech Republic; ELI
6	Corina Andronescu	Germany; Universität Duisburg-Essen
7	Ulf-Peter Apfel	Germany; Ruhr-Universität Bochum and The Fraunhofer Institute for Environmental, Safety and Energy Technology UMSICHT
8	Markus Appel	France; Institut Laue-Langevin
9	Matthias Arenz	Switzerland; University of Bern
10	Antonio Attili	United Kingdom; University of Edinburgh
11	Frank Atzler	Germany; TU Dresden
12	Alexander Auer	Germany; Max-Planck-Institut für Kohlenforschung
13	Adisa Azapagic	United Kingdom; The University of Manchester

14	Julien Bachmann	Germany; Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
15	Michael Baldea	USA; The University of Texas at Austin
16	André Bardow	Switzerland; ETH Zürich
17	Matthias Bauer	Germany; Universität Paderborn
18	Andrea Beck	Germany; Universität Stuttgart
19	Tristan Becker	Germany; TU Dresden
20	Malte Behrens	Germany; Christian-Albrechts-Universität zu Kiel
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22	Ian H. Bell	USA; The National Institute of Standards and Technology (NIST)
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24	Lorenz T. Biegler	USA; Carnegie Mellon University
25	Pegah Bineshpour	Iran; College of Engineering, University of Tehran
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27	Bastian Bloombach	Germany; Technische Universität München
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29	André L. Boehman	USA; University of Michigan
30	Benjamin Böhm	Germany; Technische Universität Darmstadt
31	Dominik Bongartz	Belgium; KU Leuven
32	Uwe Bornscheuer	Germany; University of Greifswald
33	Irina Borodina	Denmark; Technical University of Denmark
34	Michael Bortz	Germany; The Fraunhofer Institute for Industrial Mathematics ITWM
35	Christian Bressler	Germany; European X-Ray Free-Electron Laser Facility GmbH
36	Bruno Bühler	Germany; Helmholtz-Zentrum für Umweltforschung GmbH - UFZ
37	Liming Cai	China; Tongji University
38	André Casal Kulzer	Germany; Universität Stuttgart
39	Benoit Chachuat	United Kingdom; Imperial College London
40	Henry Chapman	Germany; Center for Free-Electron Laser Science
41	George Chen	China; Tsinghua University
42	Chang-Hyuck Choi	South Korea; Gwangju Institute of Science and Technology
43	Avelino Corma	Spain; Universidad de Valencia
44	Björn Corzilius	Germany; Rostock University
45	Francesco Creta	Italy; Sapienza Università di Roma
46	Gabriel J. Cuello	France; Institut Laue-Langevin
47	Alberto Cuoci	Italy; Politecnico di Milano
48	Henry Curran	Ireland; University of Galway
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54	Libor Dostal	Czech Republic; Univerzita Pardubice
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56	Matthias Drieß	Germany; Technische Universität Berlin
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58	Birgitta Ebert	Australia; The University of Queensland
59	Hellmut Eckert	Brasil; Universidade de São Paulo
60	Helmut Eichlseder	Austria; Graz University of Technology
61	Peter Eilts	Germany; Technische Universität Braunschweig
62	Andreas Erbe	Norway; Norwegian University of Science and Technology
63	Gerhard Erker	Germany; University of Münster
64	Matthias Ernst	Switzerland; ETH Zürich
65	Erik Esche	Germany; Technische Universität Berlin
66	Bastian Etzold	Germany; Technische Universität Darmstadt
67	Tiziano Faravelli	Italy; Politecnico di Milano
68	Claudio Ferdeghini	The Netherlands; Maastricht University
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71	Anna Fischer	Germany; Albert-Ludwigs-Universität Freiburg
72	Asja Fischer	Germany; Ruhr-Universität Bochum
73	Henry Fischer	France; Institut Laue-Langevin
74	Peter Fischer	Austria; Graz University of Technology
75	Amparo Galindo	United Kingdom; Imperial College London
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148	Steffen Lindner-Mehlich	Germany; Charité – Universitätsmedizin Berlin
149	John Linkhorst	Germany; Technische Universität Darmstadt
150	Gregory T. Linteris	USA; NIST
151	Alfred Ludwig	Germany; Ruhr-Universität Bochum
152	Thomas Lunkenbein	Germany; Fritz Haber Institute of the Max Planck Society
153	Ulrich Maas	Germany; Karlsruhe Institute of Technology
154	Andreas Magerl	Germany; Friedrich-Alexander-Universität Erlangen-Nürnberg
155	Detlef Markus	Germany; Physikalisch-technische Bundesanstalt
156	Holger Marschall	Germany; Technische Universität Darmstadt
157	Justus Masa	Germany; Max Planck Institute for Chemical Energy Conversion
158	Beat H. Meier	Switzerland; ETH Zürich
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160	Vera Meyer	Germany; Technische Universität Berlin
161	Carsten Meyer	Germany; Friedrich-Alexander-Universität Erlangen-Nürnberg
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188	Jens U. Repke	Germany; Technische Universität Berlin
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192	Christine Rouselle	France; Université d'Orléans
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197	Jordy Saya	The Netherlands; Maastricht University
198	Taraneh Sayadi	France; Sorbonne University
199	Thomas Scheibel	Germany; University of Bayreuth
200	Gerhard Schembecker	Germany; Technische Universität Dortmund
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203	Martin Schiemann	Germany; RU Bochum
204	Maximilian Schiffer	Germany; Technical University of Munich
205	Carsten Schilde	Germany; Technische Universität Braunschweig
206	Siegfried Schindler	Germany; Justus Liebig University Giessen
207	Hans-Joachim Schmid	Germany; Universität Paderborn

208	Wolf-Gero Schmidt	Germany; Universität Paderborn
209	Sandy Schmidt	The Netherlands; University of Groningen
210	Wolfgang Schuhmann	Germany; Ruhr-Universität Bochum
211	Christof Schulz	Germany; Universität Duisburg-Essen
212	Boelo Schuur	The Netherlands; University of Twente
213	Doris Segets	Germany; Universität Duisburg-Essen
214	Jürgen Senker	Germany; University of Bayreuth
215	Jose Serra	Spain; Universitat de València
216	Yang Shao-Horn	USA; Massachusetts Institute of Technology
217	Alexandre Simonov	Australia; Monash University Australia
218	Bart Somers	The Netherlands; TuE
219	Evan Spruijt	The Netherlands; Radboud University Nijmegen
220	T. Daniel P. Stack	USA; Stanford University
221	Dieter Stapf	Germany; Karlsruher Institut für Technologie
222	Oliver Stein	Germany; Karlsruhe Institute of Technology
223	Christoph Steinbeck	Germany; Friedrich Schiller University
224	Greg Stephanopoulos	USA; Massachusetts Institute of Technology
225	Peter Strasser	Germany; Technische Universität Berlin
226	Elena Sturm	Germany; LMU
227	Edson Ticianelli	Brasil; University of São Paulo
228	Milana Trifkovic	Canada; Univ. of Calgary
229	Philipp Trotter	Germany; University of Wuppertal
230	Angelos Tsoukalas	The Netherlands; Erasmus University Rotterdam
231	Roland Ulber	Germany; Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau
232	Gerald van den Boogart	Germany; Helmholtz-Institut Freiberg für Ressourcentechnologie
233	Luc Vervisch	France; INSA Rouen Normandie
234	Kylie Vincent	United Kingdom; University of Oxford
235	Xinfang Wang	United Kingdom; University of Birmingham
236	Peter Wasserscheid	Germany; Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
237	Hiroaki Watanabe	Japan; Fukuoka University
238	Birgit Weber	Germany; Universität Bayreuth
239	Bert Weckhuysen	The Netherlands; Universität Utrecht
240	Michael Wensing	Germany; Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
241	Charles Westbrook	USA; University of California
242	Bernd Wiedemann	Germany; Technische Universität Berlin
243	Nikolas Wöhrl	Germany; Universität Duisburg-Essen
244	Martien A. Wurdemann	The Netherlands; Maastricht University
245	Tao Zhang	China; Dalian Institute of Chemical Physics

10. Persons who are to be excluded from the Review Panel

not applicable

Signatures

Aachen, 25.01.2024

Prof. Dr.-Ing. (USA) Stefan Pischinger
(Authorised spokesperson of the managing university)

Aachen, 24.01.2024

Univ.-Prof. Dr. rer. nat. Dr. h.c. mult. Ulrich Rüdiger
(Rector of the managing university)

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