Letter of Intent

to submit a proposal for a Cluster of Excellence

# General Instructions

The Letters of Intent of the universities to submit proposals for a Cluster of Excellence are non- binding, are not reviewed and only serve to plan the review process.

Submission is requested

* for renewal proposals: by **4 pm** on **29 January 2024**.
* for establishment proposals: by **4 pm** on **15 April 2024**.

The information contained is preliminary and may differ from the actual proposal.

Please use the following template for the Letter of Intent, delete the instructions (in grey font) and convert the document to PDF format. Create a PDF file without password protection and without restrictions regarding reading, copying and printing. The PDF should be submitted via elan as “correspondence” regarding the draft proposal/establishment proposal, respectively. Please note that Letters of Intent can only be submitted by the spokespersons.

# Submission of the Letter of Intent via elan:

* + Please log in to your elan account. Only the spokesperson(s) can submit the Letter of Intent.
	+ Select “*Proposal Submission*” - “*Proposal Overview/Renewal Proposal*”.
	+ Search for the Cluster of Excellence (draft) proposal in the list and select “*Continue*”.
	+ Click the button next to “*Form for submitting comments, inquiries and additions to the DFG Head Office*” to start the online form.
	+ Upload the Letter of Intent as a PDF file and select “*Continue*”.
	+ Select “*Send*” to send the form to the DFG Head Office.
	+ You will be provided with a PDF summary of your submitted form for download and you will receive an automatic confirmation e-mail.

# 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**

[x]  Renewal proposal

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

# 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

# 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 UniversityMax Planck Institute for Chemical Energy Conversion |

# Participating Institutions

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

# Summary of the Proposal

Since the mid 20th century, the CO2 emissions associated with the use of crude oil 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 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 require a range of measures centered around the global availability of renewable energy. The resulting **de-carbonization of the energy sector** imposes challenges and opportunities for the **de-fossilization of 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 Aachen. 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. In 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 “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 CO2 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 anti-fragility**.

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** so that they fulfill all three dimensions of sustainability - ecological, economic and social?
* 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 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 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?



Figure 3: The integrated framework of the five Strategic Research Areas (SRAs) embedded
within the Competence Areas (CAs)

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.

# Principal Investigators

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | Principal investigators | Location/Institution | Field of expertise | Position |
| 1 | Jun.-Prof. Dr. phil. Katrin Arning | Aachen, RWTH | Risk Perception and Communication | W1/temporary |
| 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 |
| 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. rer. nat. Walter Leitner | Aachen, RWTH | Technical Chemistry and Petrochemistry | W3/permanent |
| Mühlheim a.d.R., MPI CEC | Molecular Catalysis |
| 12 | Prof. Dr. techn. Karl Mayrhofer | Erlangen, FZJ | Electrocatalysis  | W3/permanent |
| 13 | Prof. Dr. rer. nat. Anna Mechler | Aachen, RWTH | Electrochemical Reaction Engineering | W3/temporary |
| 14 | Prof. Alexander Mitsos, Ph.D. | Aachen, RWTH | Process Systems Engineering | W3/permanent |
| Jülich, FZJ | Energy Systems Engineering |
| 15 | Prof. Dr. rer. nat. Regina Palkovits | Aachen, RWTH | Heterogeneous Catalysis and Technical Chemistry | W3/permanent |
| 16 | Prof. Dr.-Ing. (USA) Stefan Pischinger | Aachen, RWTH | Thermodynamics of Mobile Energy Conversion Systems | W3/permanent |
| 17 | Prof. Dr.-Ing. Heinz Pitsch | Aachen, RWTH | Combustion Technology | W3/permanent |
| 18 | Prof. Dr. rer. nat. Dörte Rother  | Jülich, FZJ | Synthetic Enzyme Cascades | W3/permanent |
| 19 | Prof. Dr. rer. nat.Franziska Schoenebeck | Aachen, RWTH | Organic Chemistry | W3/permanent |
| 20 | Prof. Dr. phil. Carmen Leicht-Scholten | Aachen, RWTH | Gender and Diversity in Engineering | 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 |

# Fields of Research

|  |  |
| --- | --- |
| No. | Fields of research |
| 1 | 403-02 Technische Chemie  |
| 2 | 404-02 Technische Thermodynamik |
| 3 | 404-01 Energieverfahrenstechnik |
| 4 | 403-01 Chemische und Thermische Verfahrenstechnik |
|  | 403-04 Bioverfahrenstechnik |
| 5 | 404-04 Strömungs- und Kolbenmaschinen |
|  | 321-01 Anorganische Molekülchemie - Synthese, Charakterisierung |
| 6 | 321-02 Organische Molekülchemie - Synthese, Charakterisierung |
| 7 | 204-02 Mikrobielle Ökologie und Angewandte Mikrobiologie |
|  | 204-01 Stoffwechselphysiologie, Biochemie und Genetik der Mikroorganismen |
| 8 | 327-01 Elektronenstruktur, Dynamik, Simulation |
| 9 | 112-03 Betriebswirtschaftslehre  |
| 10 | 111-02 Empirische Sozialforschung  |

Please list up to ten disciplines primarily involved in the Cluster of Excellence, using the five- digit codes of the DFG subject structure: [www.dfg.de/en/dfg-profile/statutory-bodies/review-](https://www.dfg.de/en/dfg-profile/statutory-bodies/review-boards/structure) [boards/structure.](https://www.dfg.de/en/dfg-profile/statutory-bodies/review-boards/structure) Please prioritise entries in descending order of relevance.

# 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 Assessment and Acceptance Modelling |

# 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 | Markus Appel | France, ILL |
| 6 | Matthias Arenz | Switzerland, Universität Bern |
| 7 | Antonio Attili | United Kingdom, University of Edinburgh |
| 8 | Adisa Azapagic | United Kingdom, The University of Manchester |
| 9 | Marco Baratieri | Italy, Universität Bozen |
| 10 | André Bardow | Switzerland, ETH Zürich |
| 11 | Dirk Bartel | Germany, U Magdeburg |
| 12 | Matthias Bauer | Germany, Universität Paderborn |
| 13 | Frank Bauer | Germany, U Stuttgart |
| 14 | Andrea Beck | Germany, Universität Stuttgart |
| 15 | Malte Behrens | Germany, Universität Kiel |
| 16 | Alexis Bell | USA, Energy Biosc. Institute |
| 17 | Fabrizio Bisetti | USA, University of Texas |
| 18 | Anja Böckmann | France, IBCP Lyon |
| 19 | André L. Boehman | USA, University of Michigan |
| 20 | Benjamin Böhm | Germany, TU Darmstadt |
| 21 | Esin Ilhan Caarls | Netherlands, Eindhoven University |
| 22 | Liming Cai | China, Tongji University |
| 23 | Chang-Hyuck Choi | South Korea, Gwangju Institute of Science and Technology |
| 24 | Avelino Corma | Spain, Universidad de Valencia |
| 25 | Björn Corzilius | Germany, Rostock University |
| 26 | Francesco Creta | Italy, University of Rome |
| 27 | Gabriel J. Cuello | France, ILL |
| 28 | Alberto Cuoci | Italy, Politecnico di Milano |
| 29 | Henry Curran | Ireland, Galway University |
| 30 | Manuel Dahmen | Germany, FZJ |
| 31 | Bassam Dally | Saudi Arabia, KAUST |
| 32 | Mara de Joannon | Italy, STEMS |
| 33 | Serena deBeer |  Germany, Max Planck Institute for Chemical Energy Conversion |
| 34 | Dario R. Dekel | Israel, Technion |
| 35 | Pascale Domingo | France, INSA Rouen |
| 36 | Andreas Dreizler | Germany, TU Darmstadt |
| 37 | Hellmut Eckert |  Brasil, Universidade de São Paulo |
| 38 | Andreas Erbe | Norway, Norwegian University of Science and Technology |
| 39 | Gerhard Erker | Germany, Westfälische Wilhelms-Universität Münster |
| 40 | Matthias Ernst | Switzerland, ETH Zürich |
| 41 | Bastian Etzold | Germany, Technische Universität Darmstadt |
| 42 | Roland Faller | USA, University of California |
| 43 | Tiziano Faravelli | Italy, Politecnico di Milano |
| 44 | Ravi Fernandes | Germany, PTB |
| 45 | Federica Ferraro | Germany, TU Braunschweig |
| 46 | Anna Fischer | Germany, Albert-Ludwigs-Universität |
| 47 | Henry Fischer | France, ILL |
| 48 | Hubert Gasteiger | Germany, Technische Universität München |
| 49 | Markus Geimer | Germany, KIT |
| 50 | Roger Gläser | Germany, Universität Leipzig |
| 51 | Eirini Goudeli | Australia, University of Melbourne |
| 52 | William Green | USA, MIT |
| 53 | Temistocle Grenga | United Kingdom, Southhampton University |
| 54 | Stefan Grimme |  Germany, University of Bonn |
| 55 | Alon Grinberg Dana | Israel, Technion |
| 56 | Jan-Dierk Grunwaldt | Germany, KIT |
| 57 | Peter Güntert |  Switzerland, ETH Zürich |
| 58 | Fabien Halter | France, University of Orleans |
| 59 | Nils Hansen | USA, Sandia National Laboratories |
| 60 | Christian Hasse | Germany, TU Darmstadt |
| 61 | Marco Haumann | Germany, FAU |
| 62 | Andreas Herrmann |  Germany, DWI |
| 63 | Henner Hollert | Germany, Goethe Universität |
| 64 | Graham Hutchings | United Kingdom, Cardiff University |
| 65 | Johannes Janicka | Germany, TU Darmstadt |
| 66 | Frederic Jaouen | France, Université de Montpellier |
| 67 | Gunnar Jeschke |  Switzerland, ETH Zürich |
| 68 | Agnes Jocher | Germany, TU München |
| 69 | Yiguang Ju | USA, Princeton |
| 70 | Sebastian Kaiser | Germany, Universität Duisburg-Essen |
| 71 | Tina Kapser | Germany, Universität Paderborn |
| 72 | Jay Keasling | USA, University of California |
| 73 | Rhett Kempe | Germany, UBT |
| 74 | Andreas Kempf | Germany, Universität Duisburg-Essen |
| 75 | Berthold Kersting |  Germany, University of Leipzig |
| 76 | Reza Kholgy | Canada, Carleton University |
| 77 | Markus Klein | Germany, Universität der Bundeswehr München |
| 78 | Wolfgang Kleist | Germany, TU Kaiserslautern |
| 79 | Stephen J. Klippenstein | USA, Argonne National Laboratories |
| 80 | Katharina Kohse-Höinghaus | Germany, Uni Bielefeld |
| 81 | Marc Koper | Netherlands, Leiden University |
| 82 | Amit Kumar | Canada, University of Alberta |
| 83 | Georg Künze |  Germany, Leipzig University Medical School |
| 84 | Alexei Lapkin | United Kingdom, University of Cambridge |
| 85 | Vincent Le Chenadec | France, Gustave Eiffel University |
| 86 | Gregory T. Linteris | USA, NIST |
| 87 | Alfred Ludwig | Germany, Ruhr-Universität Bochum |
| 88 | Thomas Lunkenbein | Germany, FHI |
| 89 | Ulrich Maas | Germany, Karlsruhe Institute of Technology |
| 90 | Andreas Magerl | Germany, FAU |
| 91 | Detlef Markus | Germany, PTB |
| 92 | Beat H. Meier |  Switzerland, ETH Zürich |
| 93 | Tatiana Minav | Finnland, Tampere University |
| 94 | Micheal Mueller | USA, Princeton University |
| 95 | Graham J. Nathan | Australia, University of Adelaide |
| 96 | Daniel Pak |  Germany, Universität Siegen |
| 97 | Alessandro Parente | Belgium, Free University of Brussels |
| 98 | Brian Pauw | Germany, BAM |
| 99 | Matteo Pelucchi | Italy, Politecnico di Milano |
| 100 | Bo Persson |  Germany, FZ Jülich |
| 101 | GiovanniMaria Piccini | Italy, UNIMORE |
| 102 | Andrij Pich |  Germany, DWI |
| 103 | Martyn Poliakoff | United Kingdom, The University of Nottingham |
| 104 | Dierk Raabe | Germany, Max-Planck-Institut für Eisenforschung GmbH |
| 105 | Ortwin Renn | Germany, IASS |
| 106 | Roland Riek |  Switzerland, ETH Zürich |
| 107 | William L. Roberts | Saudi Arabia, KAUST |
| 108 | Yuri Roman | USA, Massachusetts Institute of Technology |
| 109 | S. Mani Sarathy | Saudi Arabia, KAUST |
| 110 | Philippe Sautet | USA, UCLA |
| 111 | Taraneh Sayadi | France, Sorbonne University |
| 112 | Thomas Scheibel |  Germany, University of Bayreuth |
| 113 | Viktor Scherer | Germany, RU Bochum |
| 114 | Christina Scheu | Germany, Max-Planck-Institut für Eisenforschung GmbH |
| 115 | Martin Schiemann | Germany, RU Bochum |
| 116 | Robert Schlögl | Germany, Max-Planck-Institut für Chemische Energiekonversion |
| 117 | Hans-Joachim Schmid | Germany, Universität Paderborn |
| 118 | Wolfgang Schuhmann | Germany, Ruhr-Universität |
| 119 | Christof Schulz | Germany, Universität Duisburg-Essen |
| 120 | Ferdi Schüth | Germany, Max-Planck-Institut für Kohlenforschung |
| 121 | Artur Schweidtmann | Netherlands, TU Delft |
| 122 | Jürgen Senker | Germany, UBT |
| 123 | Yang Shao-Horn | USA, Massachusetts Institute of Technology |
| 124 | Mirko Skiborowski | Germany, SVT, TU Hamburg |
| 125 | Irina Smirnova | Germany, TVT, TU Hamburg |
| 126 | Evan Spruijt |  Netherlands, Radboud University Nijmegen |
| 127 | Greg Stephanopoulos | USA, Massachusetts Institute of Technology |
| 128 | Peter Strasser | Germany, Technische Universität Berlin |
| 129 | Elena Sturm | Germany, LMU |
| 130 | Juha Tanskanen | Finland, University of Oulu |
| 131 | Edson Ticianelli | Brasil, University of São Paulo |
| 132 | Adri van Duin | USA, Pennsylvania State University |
| 133 | Toon Verstraelen | Belgium, University of Ghent |
| 134 | Luc Vervisch | France, INSA Rouen |
| 135 | Birgit Vogel-Heuser |  Germany, TU München |
| 136 | Peter Wasserscheid | Germany, FAU |
| 137 | Hiroaki Watanabe | Japan, Fukuoka Unviersity |
| 138 | Jürgen Weber |  Germany, TU Dresden |
| 139 | Bert Weckhuysen | Netherlands, Universität Utrecht |
| 140 | Charles Westbrook | USA, University of California |
| 141 | Martin Wollschläger |  Germany, TU Dresden |
| 142 | Dzmitry Zaitsau | Germany, University of Rostock |
| 143 | Tao Zhang | China, Dalian Institute of Chemical Phsysics |

# Persons who are to be excluded from the Review Panel

|  |  |  |
| --- | --- | --- |
| No. | Person | Location/Institution |
| 1 | <person> | <location, institution> |
| 2 | <person> | <location, institution> |
| 3 | <person> | <location, institution> |

# Signatures

|  |  |
| --- | --- |
| place and date | signature |
|  | name(Authorised spokesperson of the managing university) |
| place and date | signature |
|  | name(Rector / president of the managing university) |
| place and date | signature |
|  | name(Rector / president of other applicant universities) |
| place and date | signature |
|  | name(Rector / president of other applicant universities) |
| . |  |