12.10.2022 Renewal Proposal – 10 Pager Draft v0

The Fuel Science Center

„Adaptive Conversion Systems for Energy Carriers and Chemicals from Renewable Resources“

In the first funding period, the Fuel Science Center (FSC) generated fundamental knowledge as well as novel scientific methodologies, which enable the integrated conversion of renewable energy and alternative carbon sources under dynamic boundary conditions to liquid energy carriers with high energy density: Bio-hybrid Fuels. The research focuses on adaptive production and propulsion systems that enable CO_2-neutral near-to-zero pollution emission mobility. Particular emphasis was given to a holistic system assessment.

A key finding of the comprehensive system analysis is the major relevance of **Global Cross-sectoral Value Chains**. In the context of bio-hybrid fuels this is in particular the coupling of the chemical, energy and transport sector by sustainable platform molecules and their corresponding conversion systems. This results in the logical evolution of the cluster's target molecules to expand from liquid fuels alone to **Bio-hybrid Fuels & Chemicals** as enabler for a **CO_2-neutral** supply chain of all sectors with **Near-to-zero Environmental Impact**.

The corresponding resources are no longer limited to biomass and industrial CO_2 emissions, but are expanded to include all conceivable material streams such as **recycled waste**, **as well as CO_2** and **nitrogen from the air**. Thus, the value chain for the energy and the chemical sector will be supplemented by new sustainable platform molecules – fuels and chemicals - based on **non-fossil carbon**, **N_2**, and **H_2O powered by electricity from renewable resources**.

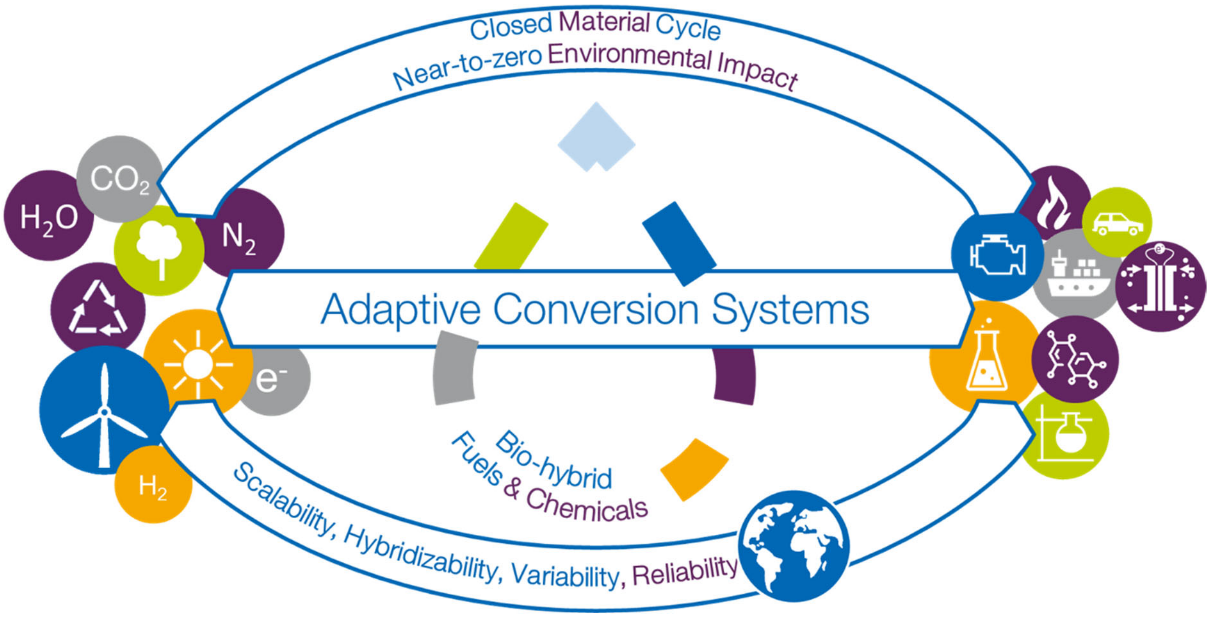
Energy conversion systems are addressed in a broader context. Thus, the energy conversion in **Internal Combustion Engines**, which has been the major subject of research so far, will be extended by (stationary) **Turbines & Burners** and electrochemical energy converters in the form of (non-H_2) **Fuel Cells**, so that all fuel-based forms of energy conversion will be covered by the FSC.

The expansion of application sectors, and the consideration of further resource streams require a confinement of the molecular diversity to molecules respectively molecule groups with the highest potential for the specific use case in terms of sustainable synthesis and application. In addition to the most promising **Bio-hybrid Fuels** identified during the current funding period, **Ammonia** from renewable resources is considered to play an important role as a carbon-free fuel and platform molecule.

Since the combustion characteristics of pure Ammonia are known to be non-favorable, the approach of the Molecularly Controlled Combustion Systems explored in the current funding period remains an important element. To cover the electrochemical processes of fuel cells this approach will be extended to **Molecularly Controlled Energy Conversion**.

With the advent of building blocks from renewable feedstocks and energy, the **process routes of the chemical industry can be re-designed** to reduce greenhouse gas emissions and simultaneously also other environmental impacts. To capitalize on this opportunity, **new molecular tools** for selective bond breaking and bond formation **as well as novel processing concepts** mastering complexity and dynamics in chemical supply chains will be developed.

The broadening of product and resource flows is accompanied by an increase in the complexity of the overall system. In addition, a **Global Competition on Renewable Resources** is to be expected, which has to be considered in the analysis of the system. The FSC takes the increased complexity into account by further strengthening the holistic systems perspective and by including all relevant **Global Material Flows** beyond the mere carbon cycle.



Generation of fundamental knowledge and novel scientific methods
for the development of
~~sustainable~~ **adaptive technical solutions**
to valorize
renewable electricity and ~~alternative carbon~~-feedstocks
~~into liquid~~ **for** energy carriers **and chemicals**
in a systems approach
~~For CO_2-neutral and near-to-zero~~
~~environmental Impact pollutant emission~~
~~propulsion and production systems.~~

Figure 1: Adapted Vision of the Fuel Science Center

Technology & System Perspective

In FSC's research, two levels of emphasis can generally be identified: On the one hand, the detailed, holistic analysis of the overall **system**. On the other hand, the in-depth transdisciplinary exploration of specific **technologies** as important building blocks for fuel science itself – both developing and establishing innovative, integrated and interconnected methods. **Transport vectors**, which enable the transport of energy and chemicals on a global scale, are at the same time the binding element between these two research levels. Ammonia and methanol in particular can be considered as major transport vectors in globally coupled energy and chemical value chains, but other hydrocarbons that can be produced on the basis of renewable resources cannot be excluded at this point.

At the system level, established technologies with a high technological maturity, such as electrolysis, direct carbon capture or the production of simple platform chemicals such as methanol or ammonia via rather conventional processes, are taken as given but considered in the system analysis. This enables research at the technology level to specifically address open questions of valorization in form of upgrading and direct use of the transport vectors. The technological improvements achieved in this way are then used in an iterative design process to optimize the overall system. While this optimization process has so far been used solely for liquid energy carriers for application in the internal combustion engine, the optimization will now be extended to multifunctional energy carriers and chemicals:

One Design Process to Fuel the Energy, Transport and Chemical Sectors

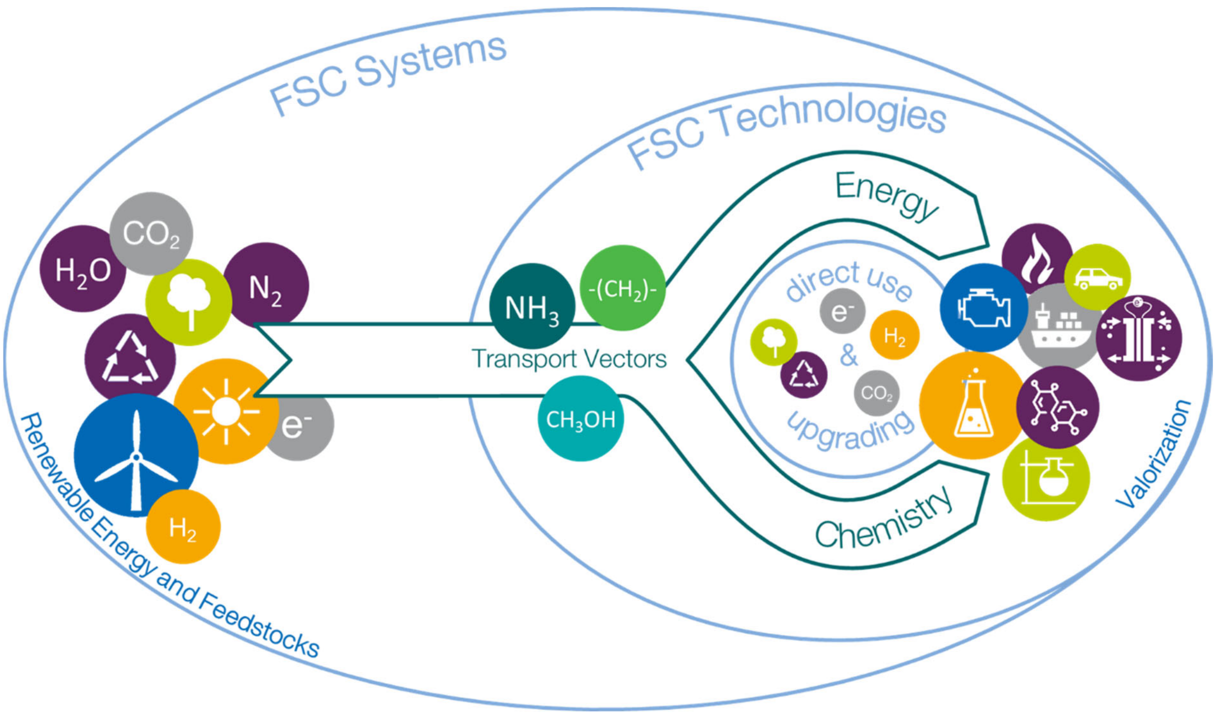


Figure 2: Adapted Mission of the FSC

With this approach, the methodological strength of the FSC established for combustion engine fuels gains greater outreach and global impact by being extended by the following key evolutions:

1. Strengthening of the holistic system perspective by considering the **Worldwide Competition on Renewable Resources** and **Global Material Flows**.
2. Extension of the cluster's target molecules to **Bio-hybrid Fuels & Chemicals** as enabler for a **CO_2-neutral** supply chain of all sectors with **Near-to-zero Environmental Impact.**
3. Extension of the energy conversion systems by **Turbines & Burners** and **Fuel Cells**, so that all fuel-based forms of energy conversion will be covered by the FSC.
4. Providing the **molecular and engineering tools** to valorize renewable feedstocks and energy for **chemical value chains of high impact**.

Research Structure & New Key Topics

The existing structural organization of the cluster into transdisciplinary Competence Areas along the different scales of length and time has proven to be advantageous, particularly with regard to the convergence of expertise from various disciplines, and will therefore be retained. So, the three Competence Areas **- (CA1) Molecular Transformations and Interactions, (CA2) Interfacial Phenomena and Devices, (CA3) Fuel Design and Sustainable Cross-sectorial Value Chains -** remain the scientific backbone of the FSC comprising the individual creativity, methodological expertise, and institutional infrastructure of the involved Principle Investigators (PIs).

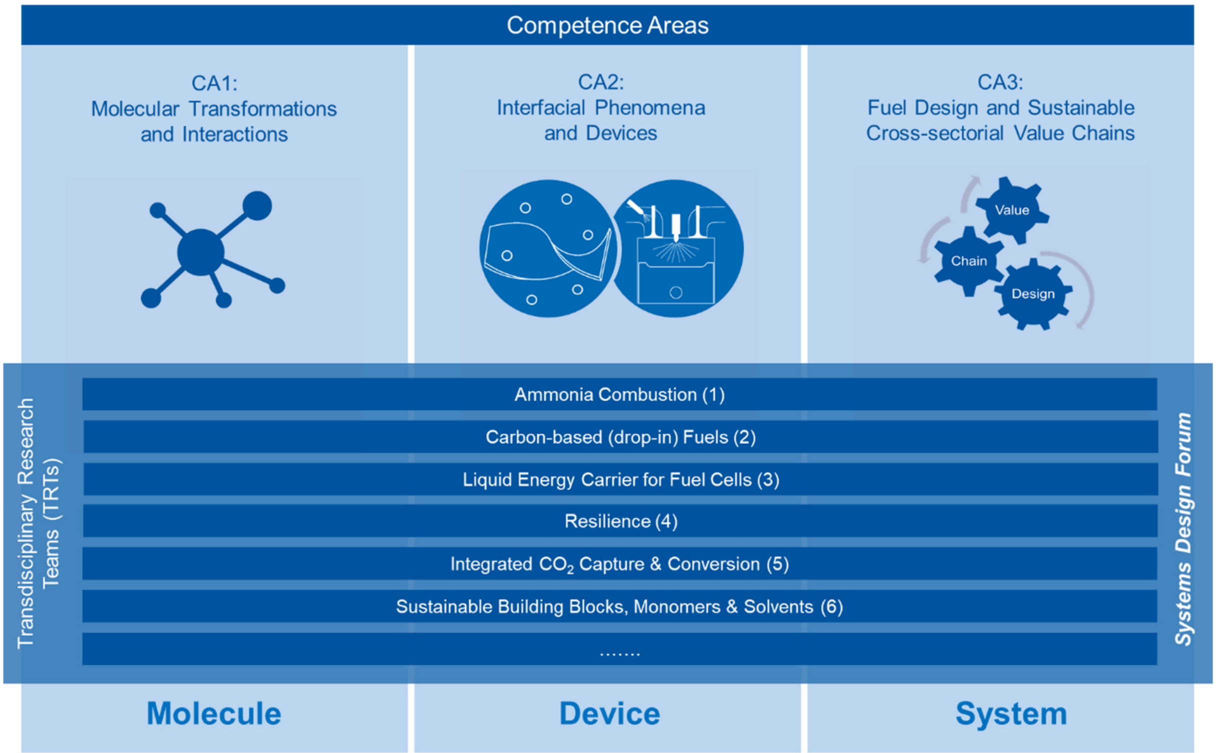


Figure 3: FSC Research Structure

In addition, the interdisciplinary integration of research is to be strengthened through further key topics along the competence areas. The following six key topics were identified as logical evolutions of the FSC.

1 Ammonia Combustion

PIs: Boxx, Eichel, Heufer, Khetan, Kneer, Kunz , Leonhard, Linkhorst*, Palkovits, Pischinger, Pitsch, Schmitz, Schröder, Simon, Wessling*

An important building block of global material flows based on renewable energy will be ammonia (NH_3) - both as a platform chemical for the chemical industry and as a carbon-free fuel for the transportation sector. Up to now, it has been produced almost exclusively via the Haber-Bosch process based on fossil resources. Alternative ammonia synthesis technologies themselves are already the subject of current research and are therefore not seen as an innovative research focus for the next phase of FSC. The cross-sectoral integration of nitrogen respectively ammonia into global value chains, on the other hand, appears to be a logical enhancement of the clusters holistic research approach.

NH_3 can serve as an energy carrier in both fuel cells and internal combustion engines. In addition to the electrochemical experiments of key topic 3, the combustion of NH_3 is therefore to be investigated in detail along all scales reaching from fundamental kinetics, combustion system development to the assessment of the sustainability of NH_3 pathways.

With the increasing relevance of completely CO_2-free energy conversion, carbon-free fuels such as ammonia are coming into focus. Some general fuel properties of ammonia in comparison to diesel and other alternative fuel candidates are summarized in Table 1.

The ignition temperature is the highest and the flammability limits are the narrowest for ammonia compared to the fuels in Table 1. As a consequence, ammonia is reluctant to combustion and requires special measures to allow an efficient and clean combustion. What might be beneficial to suppress unwanted combustion phenomena (knocking) in spark ignited combustion systems, diffusive combustion of ammonia is only possible with supportive measures as e.g. a pilot injection of a high reactivity fuel.

	Diesel (liq.)	Methanol (liq., 65°C)	Ammonia (liq., -33°C)	Hydrogen (liq., -253°C)
Lower Heating Value in MJ/kg	42.7	19.7	18.6	120
Adiabatic Flame Temperature in °C	2030	1880	1800	2110
Ignition Temperature in °C	≥ 225	440	630	560
Lower / Upper Flammability Limit Vol.-%	0.6 / 6.5	6 / 50	14 / 32.5	4 / 77
Laminar flame speed in m/s (λ = 1, T ≈ 300 K, p = 1 bar)	0.48 (n-heptan)	0.4	0.07	2.7

Table 1: *Fuel properties of ammonia and other alternative fuel candidates compared to Diesel*

As already indicated by the narrow flammability limits, the laminar flame speed of ammonia is very low as well. Hence, the combustion system needs supportive measures to increase the flame speed for efficient combustion. One approach is to utilize ammonia as low reactivity fuel in FSC's Molecular Controlled Combustion Systems (Dual Fuel & Pre-Chamber) for example in combination with hydrogen or (e-)methane as high reactivity fuel. Fundamental understanding of the combustion and emission characteristics have to be gained, particularly since non-linear behavior can be expected for dual fuel combustion. Here, the well established FSC tool chain consisting of fundamental experiments such as Rapid Compression Machine

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**Co-PI/Junior Research Group Leader | Main Responsible PI | (potential new PI)*

& Shock Tube in combination with detailed kinetic modelling, the simulation and experimental validation of emission formation up to single-cylinder engine experiments is applied to design a highly efficient and clean combustion system.

In context of combined NH_3/H_2 combustion systems, the potential of integrated on-board NH_3 reforming has to be evaluated. Besides the fundamental kinetics of the (electro-) chemical and/or thermal reforming, the reactor process design and mixture formation as well as the heat integration of such a system coupled to the exhaust aftertreatment has to be understood in detail.

As observed for hydrogen combustion systems, it can be expected that the interaction between NH_3(+H_2) and engine oil has negative impact on the tribology of the internal combustion engine. To evaluate potential tribology effects, the respective FSC tool chain consisting of wear experiments is applied.

2 Carbon-based (Drop-in) Fuels

PIs: Arning, Boxx, Du, Heufer, Jupke, Kneer, Leonhard, Mitsos, Palkovits, Pischinger, Pitsch, Roß-Nickoll, Schmitz, Schröder, Simon, Venghaus, von der Aßen, Ziefle*

So far, the research focus has been on the application of liquid, CO_2-neutral fuels in novel molecularly controlled combustion systems. This approach will be expanded to new fuel candidates but, more importantly, to the most relevant fuel candidates for the medium to long term perspective in both new and established energy conversion systems. The latter means a consolidation of the bio-hybrid fuels already identified and, in the process, a reduction of the molecular diversity as well as the targeted exploitation of further fuel candidates and fuel blends that are compatible with the current vehicle fleet.

Such fuels should at the same time offer backward compatibility with today's applications and legislation, as well as significant potential for improvement in terms of increased efficiency and zero-impact pollutant emissions in new combustion processes. For example, it has already been shown that the combination of longer-chain alcohols (C5-C10) with alkanes results in a drop-in-capable diesel fuel with considerable soot reduction potential without further adjustments to the power train. Adjusting the engine calibration offers further potential for reducing nitrogen oxide emissions and increasing efficiency. Finally, further potential can be raised by modifying the engine hardware and dedicated, optimized new combustion engines and exhaust aftertreatment systems.

The challenge of these cascaded yet tide fuel requirements defined by both fleet compatibility as well as legislation is addressed by an adaptive multi-component fuel design process. With regard to the application of these fuels in existing vehicles, fuel infrastructure and society sensitized to energy and sustainability, tribological effects, toxicity and acceptance are of particular importance and have to be considered in the fuel design process in addition to the combustion properties.

The FSC's broad database is particularly important in this key topic, which is why hybrid AI methods coupled to the overarching FDM concept must be further developed to make optimal use of it.

The defossilization of the existing vehicle fleet poses a particular challenge, especially in relation to the global demand for large quantities of CO_2-neutral fuels in the shortest possible time. One bottleneck is the upscaling of promising processes to relevant scales. This challenge is to be addressed by virtual upscaling, with which the potential of new synthesis pathways for a large-scale application can be identified at an early stage of development on both, technology and system level.

3 Liquid Energy Carrier for Fuel Cells

PIs: Boxx, Du, Eichel, Keller*, Kneer, Kunz*, Lauterbach, Mechler, Palkovits, Pischinger, Schmitz, von der Aßen, Wessling, Zobel*

Non-H_2 fuel cells or direct liquid fuel cells (DLFC) show great potential as energy conversion systems with zero or near-to-zero environmental impact. DFLCs share a variety of advantages to the currently more prominent hydrogen fuels cells: superior theoretical energy density, variable modes of configuration, immediate load response and comparably simple fuel systems, which could be compatible with the existing infrastructure.

Generally, DLFC fuels can be divided into alcoholic and other fuels (Figure 4). The most advanced DLFC is methanol based and already commercially available. Other fuels under investigation are ethanol, 2-propanol, glycol, acids, and nitrogen-based fuels such as ammonia.

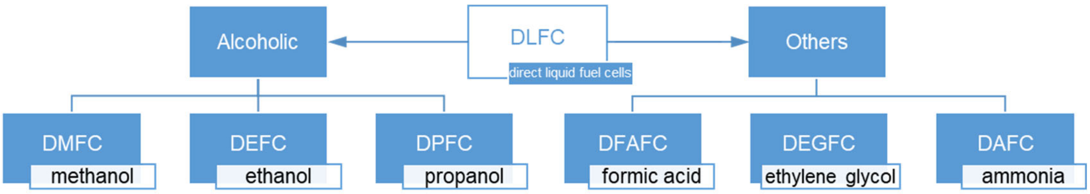


Figure 4: *Overview of DLFCs as alternatives to "conventional" H_2-based fuel cells in mobile or stationary applications.*

The main challenge of DLFCs is their high cost caused by the high loading of anode catalyst to achieve power densities comparable to hydrogen fuel cells. Another challenge is to find a suitable cathode catalyst that selectively allows the oxygen reduction reaction (ORR) and avoids fuel oxidation; such a catalyst is not yet available.

In particular, fuel design for liquid fuel cells represents an important new field of research. In preparation, an initial literature review has already been conducted as part of an FSC internal Flex Fund project. This is now to be extended and substantiated with the first basic electrochemical experiments. The experimental investigations will be accompanied by a system analysis at stack level and a life cycle assessment.

Methodologically, the extension of the topic to fuel cells also represents a logical evolution of the FSC. The most important interdisciplinary competences from the areas of catalysis and electrochemistry, membrane and electrode design accompanied by innovative analysis methods such as in-situ spectroscopy, right through to system integration and life cycle assessment are already represented in the FSC, so that the holistic, iterative optimization approach established in the FSC can directly be applied.

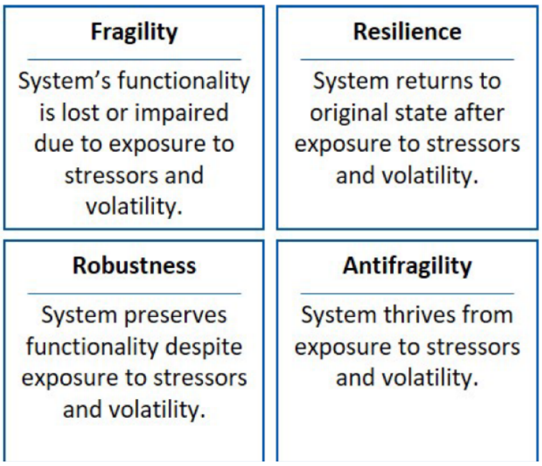
4 Resilience

PIs: Arning, Du, Jupke, Mitsos, Roß-Nickoll, Venghaus, von der Aßen, Walther, Ziefle*

The research orientation of the Cluster of Excellence is characterized by a high degree of adaptivity to current societal challenges. With global warming as the overarching driver for research into sustainable mobility solutions, the FSC has always recognized and addressed linked problems such as the food vs. fuel challenge and the diversification of sustainable resources at an early stage. In the current crisis, the coupling of the energy, transport and chemical sectors and their importance for a resilient global economy becomes particularly clear. The dependence on fossil resources from few individual countries, specialized technologies and limited transport pathways are mainly responsible for the vulnerability of the existing system.

With the aim of designing a resilient, or rather antifragile (see Figure 5), Conversion Systems for Energy Carriers and Chemicals from Renewable Resources, the models of the FSC are extended to include stress and volatility indication at the global level. In this context, modelling approaches for complex ecological systems are to be transferred to human-made economic systems.

One challenge in modelling complex global systems is the integration of innovative technologies for which there is little to no data on their application at relevant scales. This is where the FSC's strength comes into play: it can model new technology components at an early stage of development and thus integrate them into the overall system using the extensive FSC database. Analogous to key theme 2, a virtual upscaling of new process paths must therefore take place, considering volatile political, ecological and social boundary conditions.



Fragility

System's functionality is lost or impaired due to exposure to stressors and volatility.

Resilience

System returns to original state after exposure to stressors and volatility.

Robustness

System preserves functionality despite exposure to stressors and volatility.

Antifragility

System thrives from exposure to stressors and volatility.

Figure 5: Definition of Stability Descriptors

5 Integrated CO_2 Capture & Conversion

PIs: Blank, Bolm, (DeBeer), Eichel, Jupke, Keller, Khetan, Klankermayer, Kunz*, Lauterbach, Leitner, Leonhard, Linkhorst*, Mechler, Mitsos, Palkovits, Rother, Schüth, Simon, (Tüysüz), von der Aßen, (Vorholt), Wessling, Zobel*

The current approach of bio-hybrid fuels as integrated (electro)-catalytic transformations of biomass and CO_2 into fuel molecules is to be extended to the dynamic integrated capture and conversion of CO_2 in general in order to increase the efficiency compared to the individual, separate steps. This explicitly excludes the direct capture of CO_2 from air, as this is already practiced on a relevant scale, but rather the upgrading of the transport vectors (cf. Figure 2 right hand side) to various product molecules. As a consequence, there is a close link to the other key topics (drop-in fuels, monomers, solvents, ...) via the targeted molecules.

In order to define the optimal degree of integration and determine the efficiency of capture and conversion, a detailed understanding of the molecular pathways and mechanisms is necessary. This requires the development of new experimental and numerical methods in the different length and time scales. On molecularly level a theoretical design approach is envisaged to discover suitable catalytic material and determine requirements for variable C sources in quality and quantity.

Of particular interest is the energy input into the capture and conversion process. In addition to conventional approaches, various innovative methods for energy input into (bio-)chemical/catalytic processes (mechanical, microwaves, photons, ...) are already being investigated in ongoing FSC projects. The task here is to identify tailor-made solutions for the dynamically operated, integrated capture and conversion process and evaluate them from laboratory scale to large-scale application.

6 Sustainable Building Blocks, Monomers & Solvents

PIs: Blank, Bolm, (DeBeer), Du, Eichel, (Herres-Pawlis), Jupke, Keller*, Khetan, Klankermayer, Kunz*, Lauterbach, Leitner, Leonhard, (Leonori), Linkhorst*, Mechler, Mitsos, (Piccini), Palkovits, Rother, Simon, Schoenebeck, Schüth, (Schwaneberg), (Tüysüz), von der Aßen, Walther, Wessling, Zobel*

The envisaged system design approach requires an expansion of the product range. Of course, the complete range of the chemical industry cannot be represented in technological depth. Rather, the focus should be on the essential building blocks, monomers and solvents as the "main branches" of a new and sustainable "chemist-tree" rooted in multifunctional energy carriers, integrated captured CO_2, biomass and recycled material flows. In addition to new synthesis paths to known product molecules, new molecules with better properties are also being considered, in which for example biodegradability is already considered in the molecular design process of the building blocks via bond cleavage. This is an approach that shows strong analogies to the well-established fuel design process, where the "splitting", i.e. the combustion, of the molecules is already incorporated as an optimization parameter in the fuel synthesis. As a further analogy to the current approach, adaptability to fluctuating resource flows remains an important requirement. In this way, all competence areas are also included in this key topic, from molecular transformation to adaptive multiphase reactor design to the modelling of feedstock availability and supply chain flexibility in a global system perspective.

Supporting Structures

The main measures of the supporting structures specific to FSC remain support of early career researchers and equal opportunity, management, quality assurance, and public engagement. While the FSC has already been able to successfully implement the planned measures in relation to the promotion of young researchers, quality assurance and public engagement, there is still potential for improvement, particularly in relation to equal opportunity. This potential weakness was recognized early on and counteracted with priority projects funded through flexible funds. In detail, the FSC is now accompanied by Prof. Leicht-Scholten as a new PI in the area of gender and diversity through a dedicated project, analogous to the Cluster of Excellence „Internet of Production“ (IoP).