The Integrated Fuel & Chemical Science Center

Adaptive Conversion Systems for Sustainable Energy Carriers and Chemicals

Renewal Proposal EXC2186

DFG Deutsche Forschungsgemeinschaft
German Research Foundation

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Confidential!

We kindly ask that all content shared in this meeting be treated with the utmost confidentiality. Your cooperation is greatly appreciated.
If anyone feels a conflict due to another cooperation or obligation, we respectfully ask you to excuse yourself from this session.

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Guiding Questions for the Discussion

1. Are the Vision & Mission Well-Articulated?
   - Does the mission statement of the research program clearly define its goals and purpose?
   - Are the objectives of the research program aligned with the overall mission and vision?
2. Is the Structure of the Research Program Sound?
   - Do the Strategic Research Areas (SRAs) provide a logical and coherent structure that supports our goals?
   - Are the different components of the program well-integrated and do they effectively contribute to the overall success?
3. Is the Research Initiative Sufficiently Motivated?
   - Have we provided a strong and compelling rationale for the research initiative?
   - Do the proposed research questions address significant gaps or needs in the current knowledge?
4. Are There Any Creative and Innovative Suggestions for Supporting Activities?
   - What additional strategies can we employ to enhance the visibility and impact of the research program through public engagement and outreach?
   - How can we improve our efforts in nurturing young talent and fostering the next generation of researchers within the program?
   - Are there innovative approaches to knowledge transfer and collaboration that we should consider incorporating into our activities?

GLOBAL GREENHOUSE GAS EMISSIONS BY SECTOR 2019

Update figures

49.76 Gt/a CO_2eq

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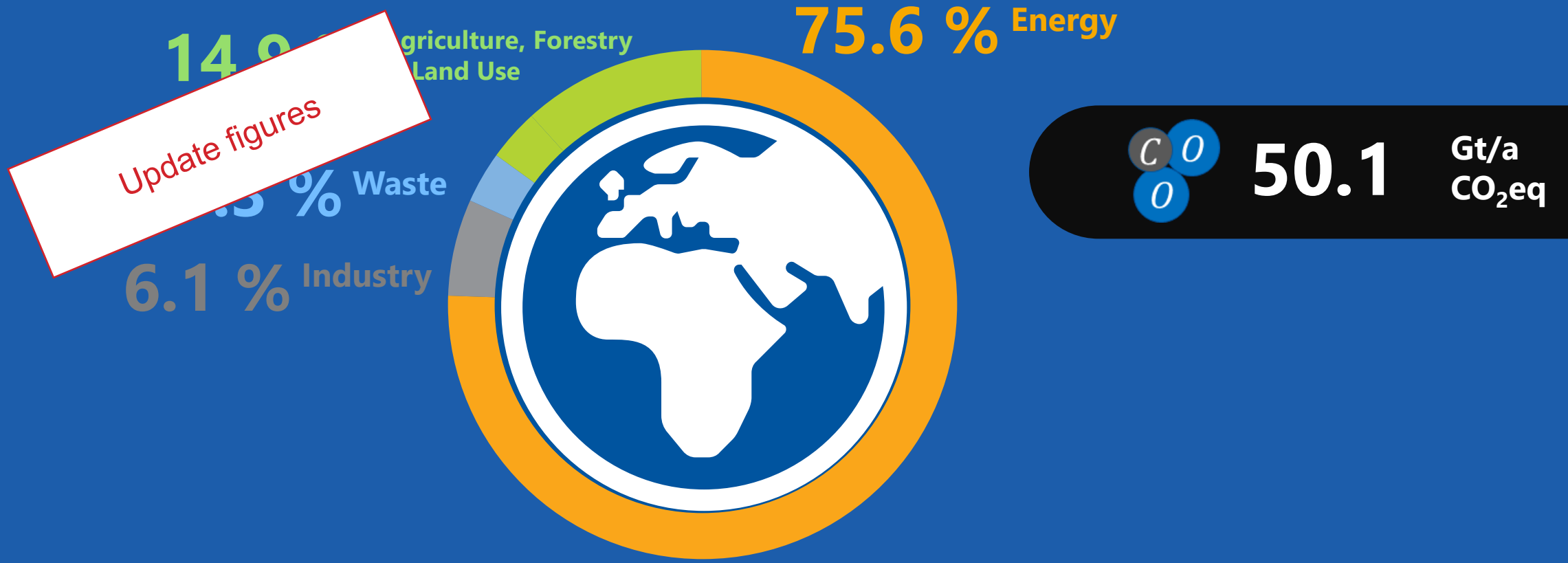
GLOBAL GREENHOUSE GAS EMISSIONS BY SECTOR 2019



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GLOBAL GREENHOUSE GAS EMISSIONS BY SECTOR 2019

14.9 % Agriculture, Forestry & Land Use

75.6 % Energy

3.3 % Waste

6.1 % Industry

TRANSPORT 17.0%

49.76 Gt/a CO_2eq

8.4 Gt/a CO_2eq

Chemistry?

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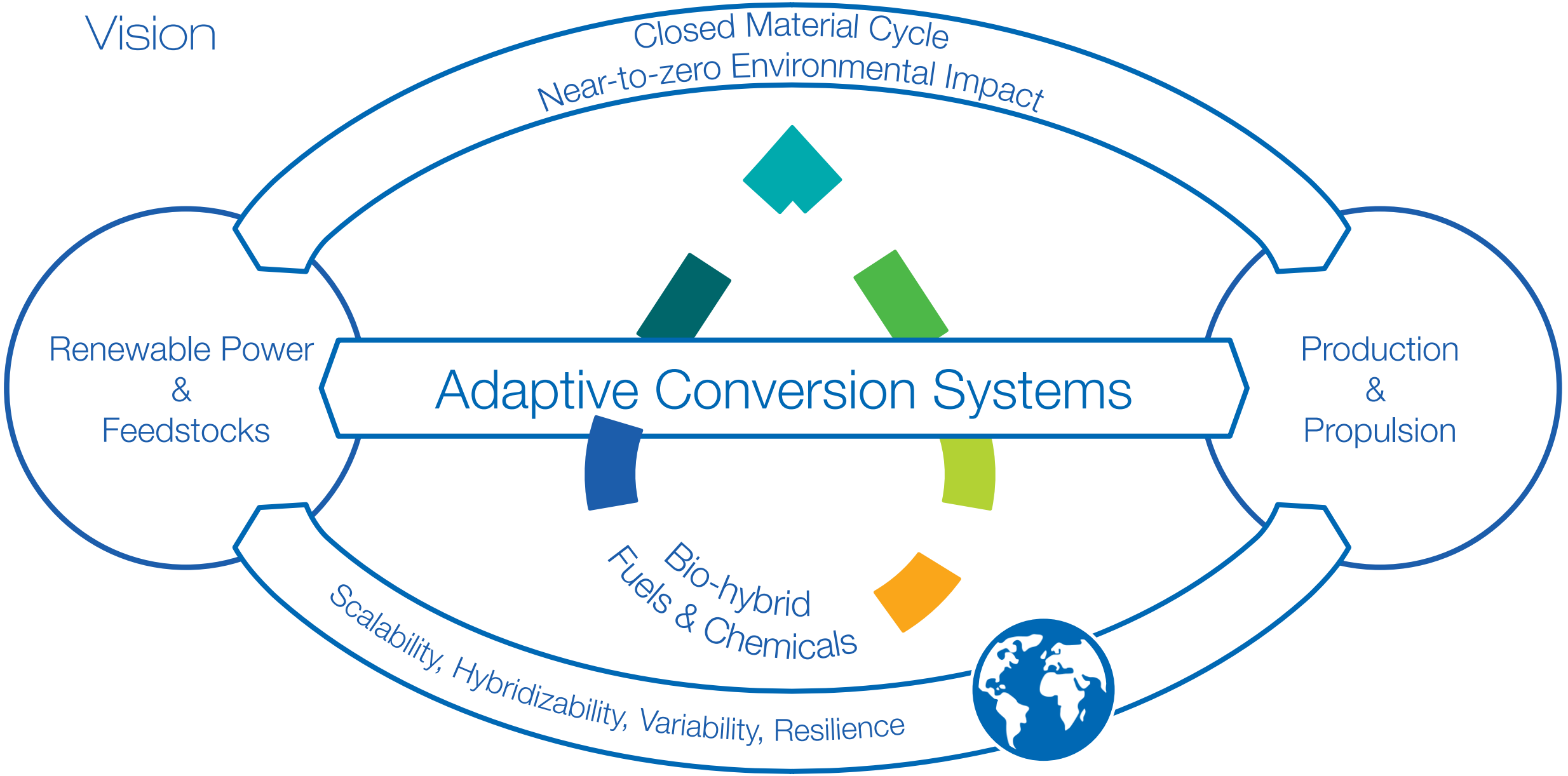
Vision



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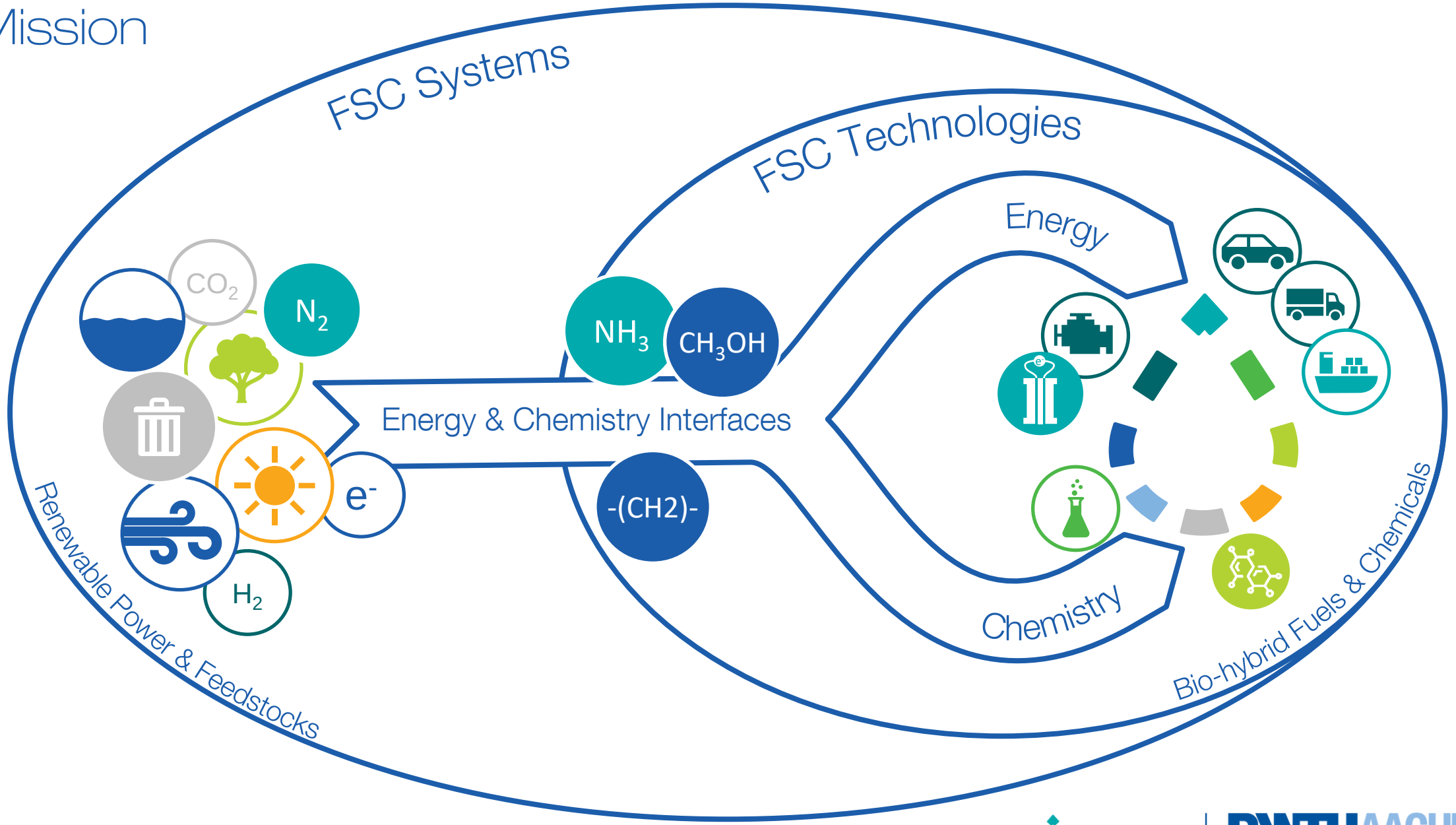
Mission



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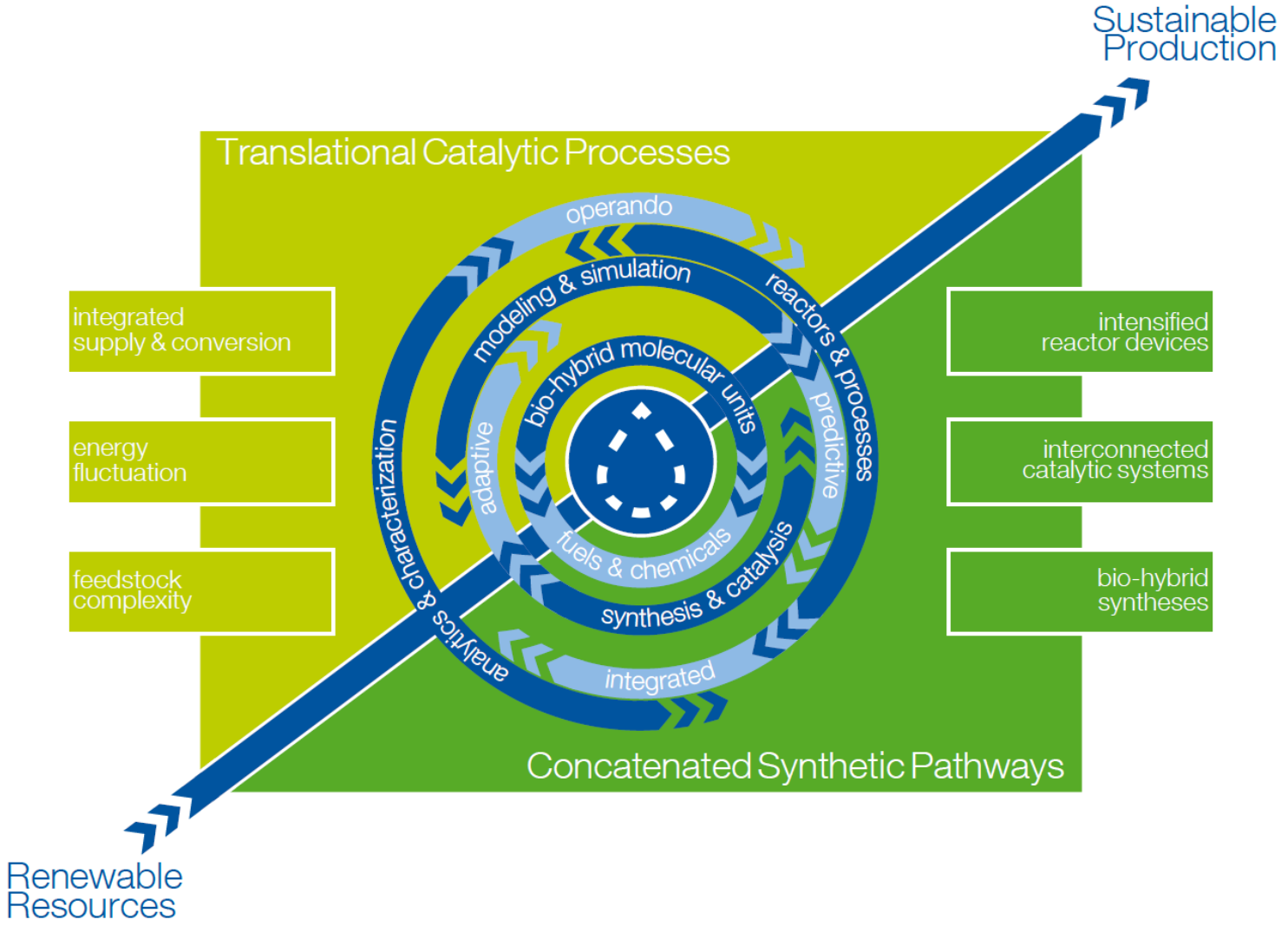
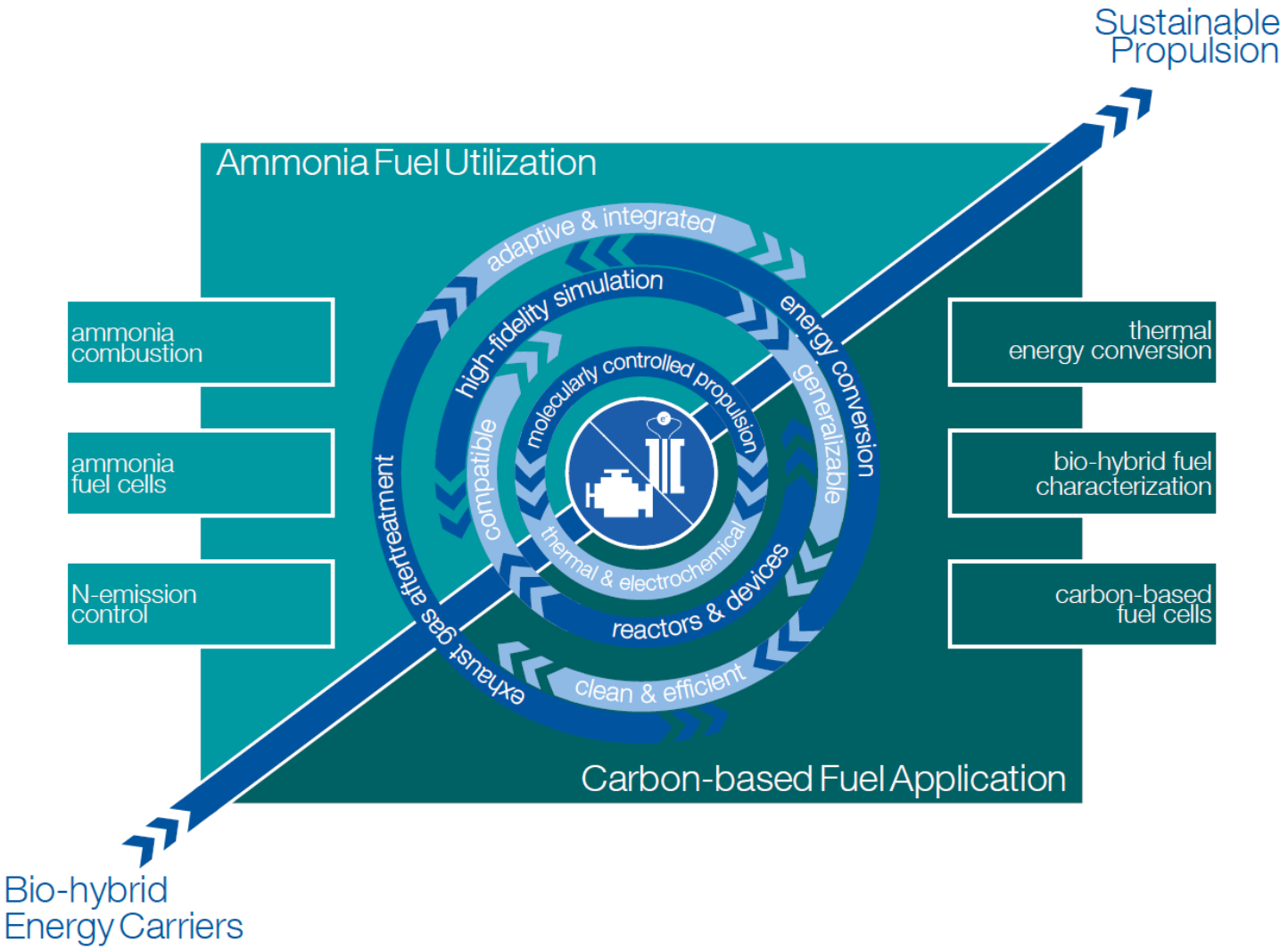
Scientific Objectives - Production

Exploration of chemo-, bio- and electro-catalytic pathways for the selective formation of C-H, C-C, C-O, and C-N bonds from renewable resources with the aim to integrate the individual transformations into optimized synthetic pathways for fuels and chemicals (concatenation) and their validation in view of feedstock variation and energy fluctuation in post-fossil value chains (translation).

Advancing the toolbox in experiment and theory for the investigation of complex catalytic reactions and processes to derive design principles from the molecular to the process level as input for and in response to the interdisciplinary analysis in the Fuel & Chemical Design Forum.



Scientific Objectives - Propulsion



Mitigate carbon emissions from existing vehicle fleet by developing bio-hybrid fuel based molecularly-controlled engine concepts that can be retrofitted to existing combustion systems enabled through advanced technologies for combustion and aftertreatment systems with energy conversion efficiencies beyond 50 % and near-zero pollutant emissions.

Develop carbon- and ammonia-based fuel cell concepts and ammonia-fueled combustion engines for new passenger vehicles, heady-duty, and marine applications enabled by fundamental understanding of the involved thermochemical and electrochemical processes

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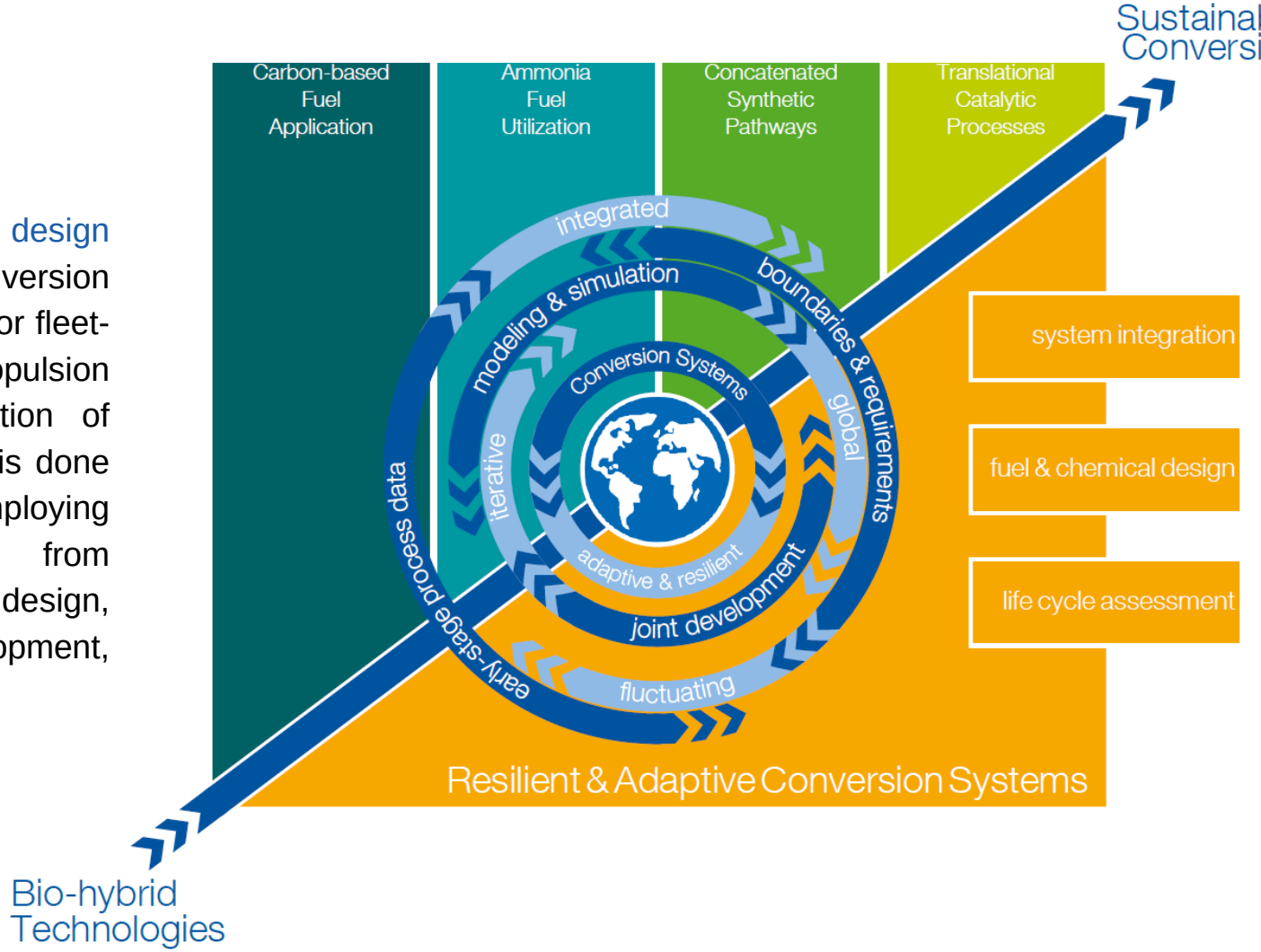
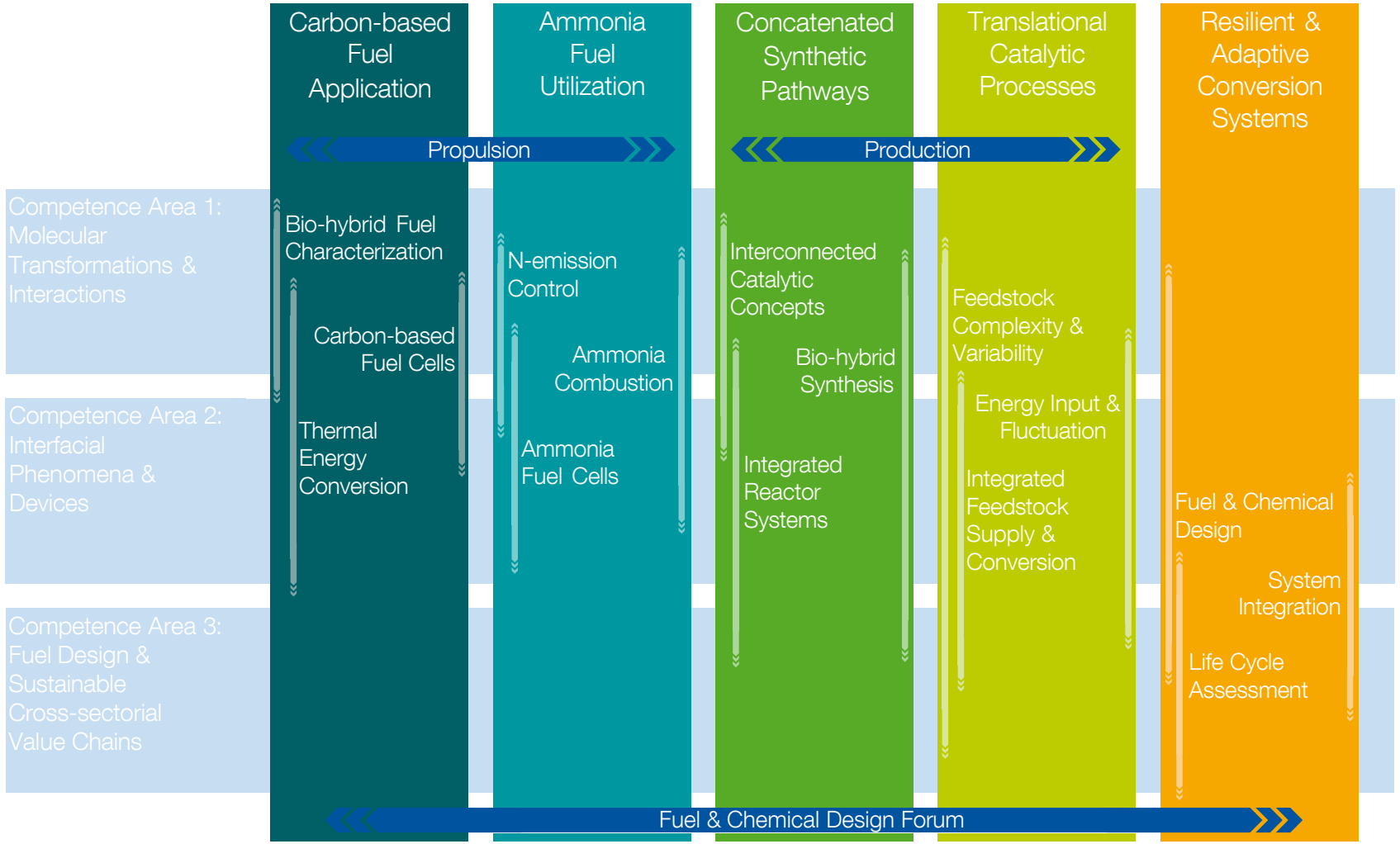
Scientific Objectives - System

The fuel and chemical design optimizes the overall conversion performance, accounting for fleet-compatible and novel propulsion concepts and co-production of chemicals and fuels; this is done by developing and employing cutting-edge methods from propulsion equipment design, production process development, and machine learning.



System integration of the developed fuels, processes and pathways is enabled by interdisciplinary assessment and optimization of resilient and adaptive intersectoral conversion systems based on systemic risks, stakeholder perspectives, policies and sustainability criteria.

Structure of the Research Program: Strategic Research Areas Extend Across all Competence Areas



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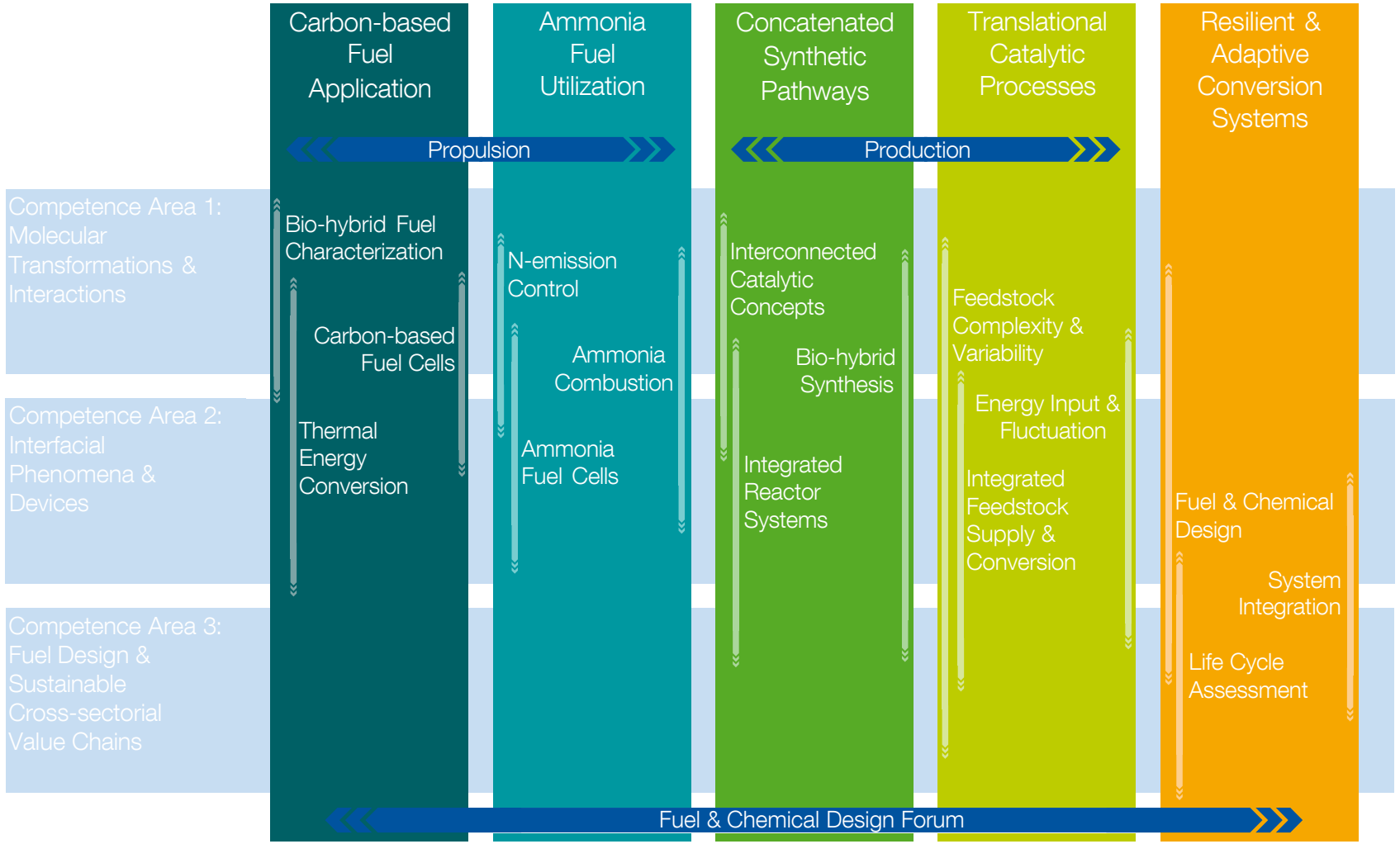
Structure of the Research Program: Strategic Research Areas Extend Across all Competence Areas



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Strategic Research Area I: Carbon-based Fuel Application
Molecularly Controlled Propulsion Systems

Carbon-based Fuel Application

Bio-hybrid Fuel Characterization

Carbon-based Fuel Cells

Thermal Energy Conversion

Molecularly Controlled Combustion

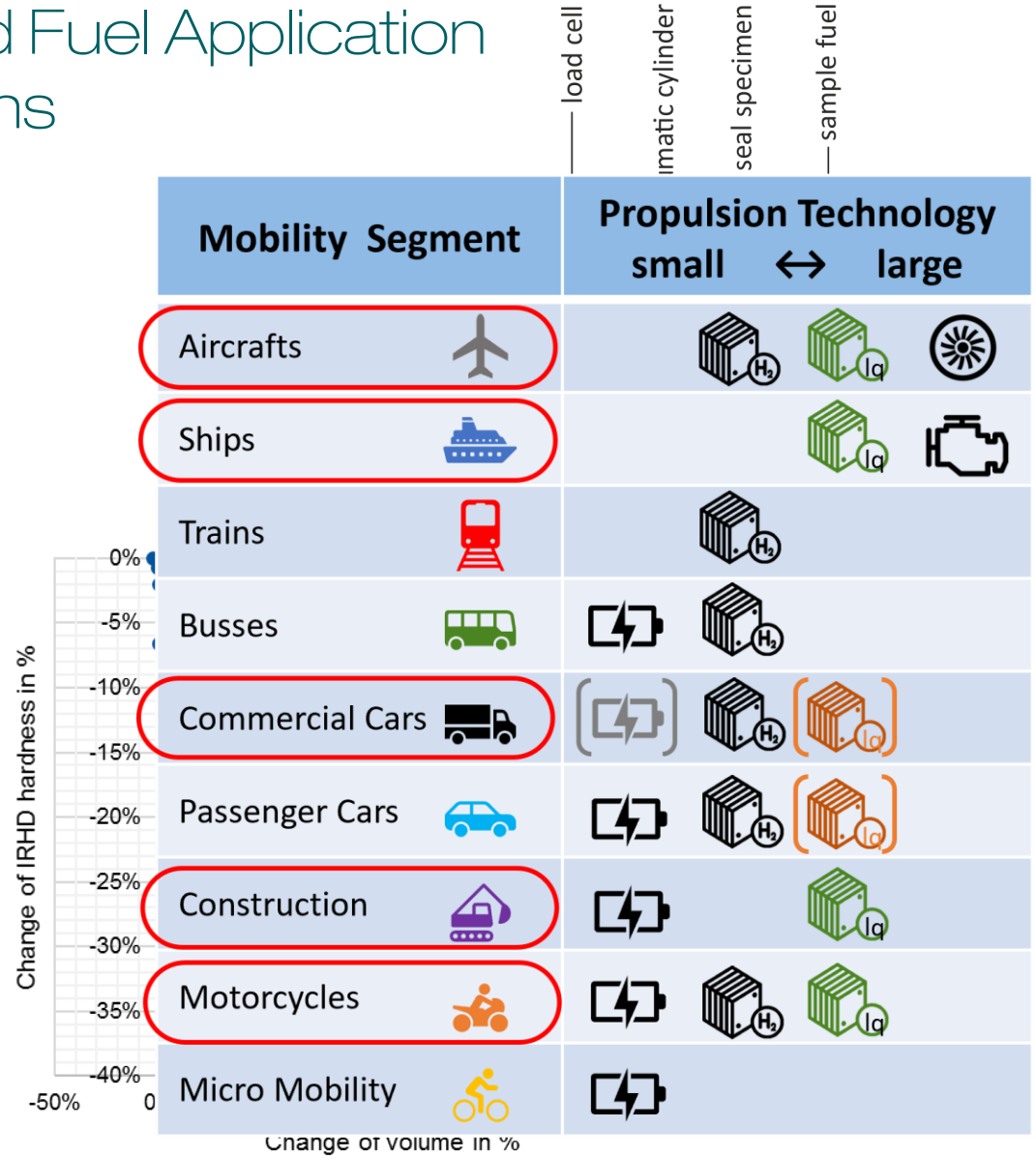
molecular torch & spark
in-cylinder coating
adaptive exhaust gas aftertreatment

Fuel & Device Compatibility

combustion characteristics
tribology & elastohydrodynamics
long-term behavior
via accelerated testing & simulation

Fuel Cell Technologies

low- & high-temperature
flex-fuel
dynamic operation



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Strategic Research Area I: Carbon-based Fuel Application
Mastering Complexity of Chemical Kinetics

Carbon-based Fuel Application

Bio-hybrid Fuel Characterization

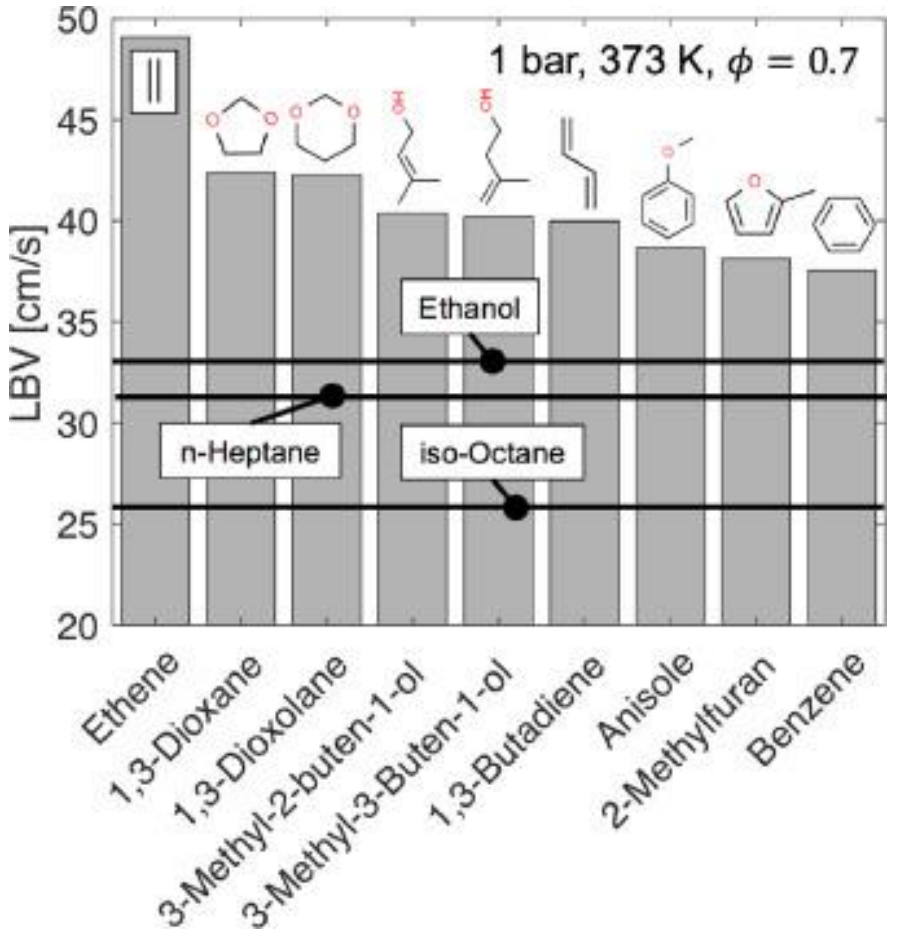
Carbon-based Fuel Cells

Thermal Energy Conversion

Objectives

- devise and implement new numerical and experimental methods to determine the reaction network, thermodynamic, and process performance of bio-hybrid fuels that facilitate an machine learning (ML) assisted Fuel & Chemical Design Process

- The exploration of universal differential equations (UDE) and natural language processing (NLP) techniques for kinetic model development and the integration of such ML approaches in established tools like FSC-tool ChemTraYzer (CTY) shall enable superior accuracy, generalizability, high computational efficiency, discovery of missing reactions, high-quality datasets, and improved parallelized training strategies.



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Strategic Research Area I: Carbon-based Fuel Application
Fleet Compatible Fuel and Engine Co-optimization

Carbon-based Fuel Application

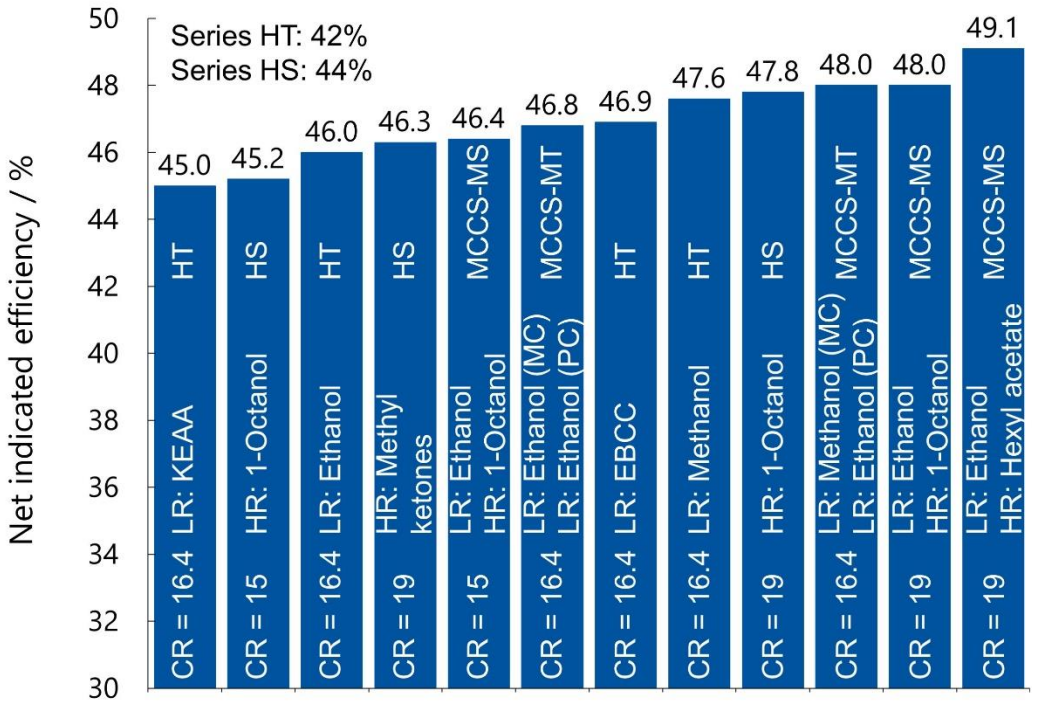
Bio-hybrid Fuel Characterization

Carbon-based Fuel Cells

Thermal Energy Conversion

Objectives

- identify bio-hybrid fuels and fuel blends that are compatible with the existing vehicle fleet
- co-develop a highly adaptive molecularly controlled propulsion system design, yielding an indicated efficiency of $\eta_i > 50$ % for on-road passenger cars
- enable a zero-impact emission strategy by combining the molecularly controlled propulsion system with a tailored and adaptive exhaust gas aftertreatment system, despite the restrictions of fleet compatibility fuel and limited hardware modifications



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Strategic Research Area I: Carbon-based Fuel Application
Next Generation Direct Liquid Fuel Cells

Carbon-based Fuel Application

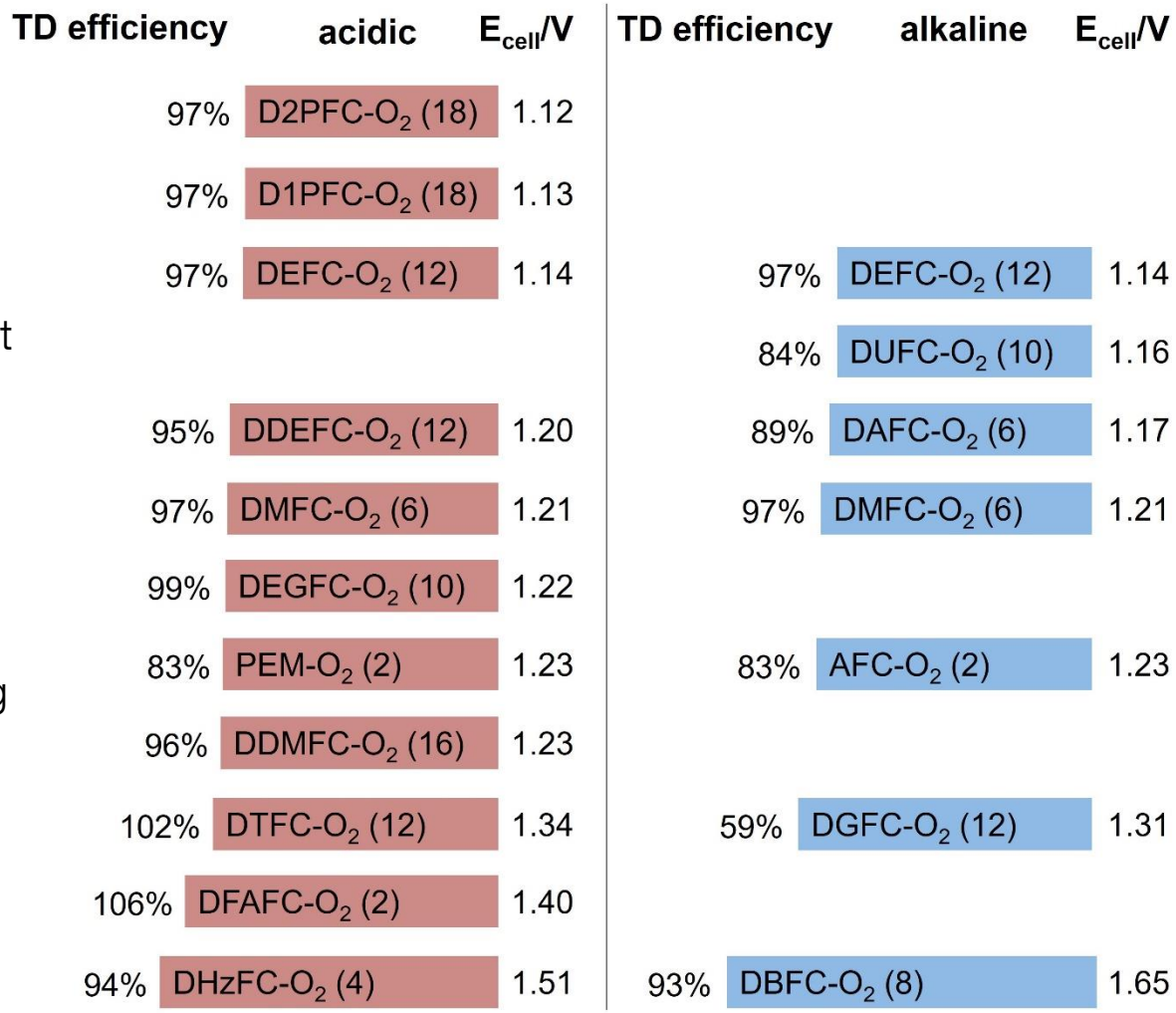
Bio-hybrid Fuel Characterization

Carbon-based Fuel Cells

Thermal Energy Conversion

Objectives

- develop adaptive fuel cells that can work with a variety of fuels and their blends,
- optimize fuel conversion by tailored fuel-catalyst interactions, screening new catalyst materials but also the fuel itself
- optimize membranes for higher stability, reduced fuel cross-over without losses in the high ionic transport performance
- study and mitigate degradation effects by in-depth structural analysis as well as optimized operation strategies and showing their feasibility on the system level



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Strategic Research Area II: Ammonia Fuel Utilization
Carbon-free, Clean & Efficient Energy Conversion

Ammonia Fuel Utilization

N-emission Control

Ammonia Combustion

Ammonia Fuel Cells

Molecularly Controlled Combustion

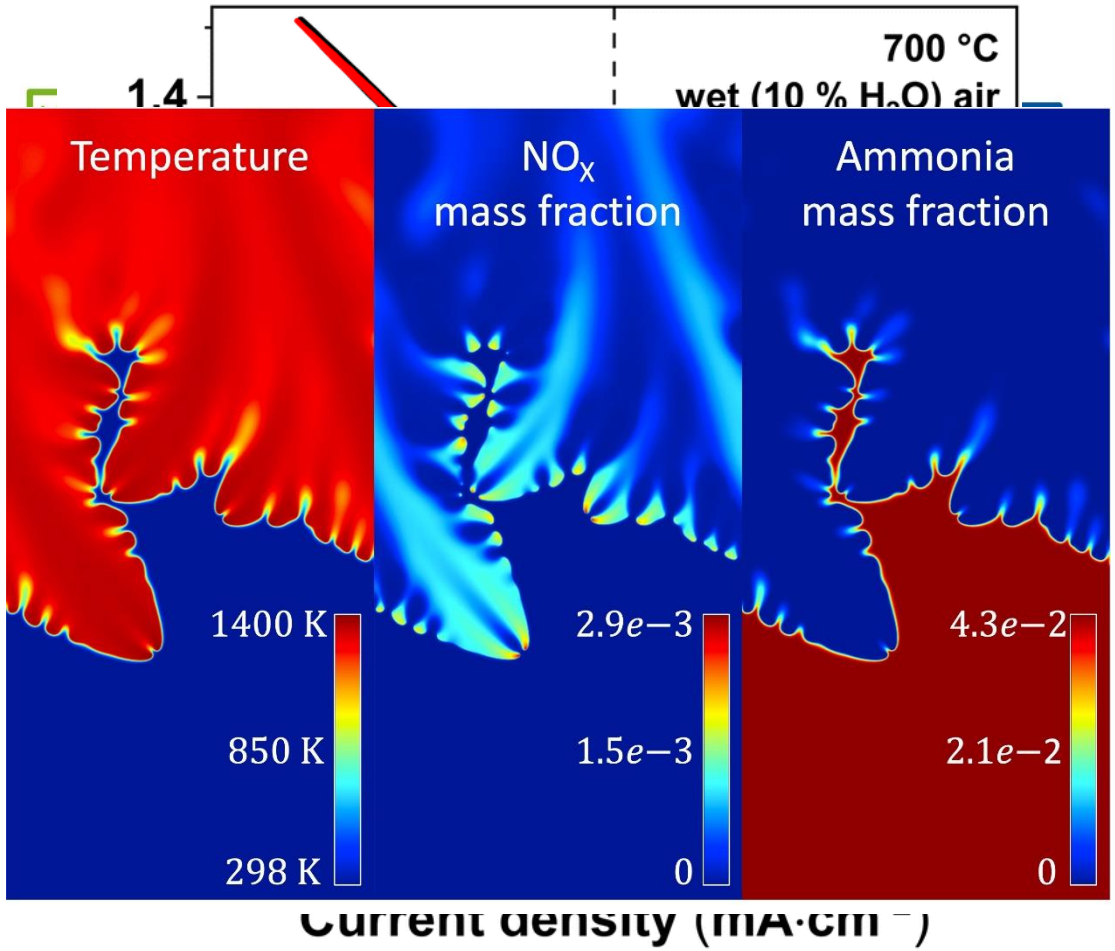
molecular torch & spark
in-cylinder coating
adaptive exhaust gas aftertreatment
reactivity tailoring

Fuel & Device Compatibility

internal reforming
injection technology
material interaction

Fuel Cell Technologies

low- & high-temperature
proton-conducting SOFC
non nobel-metal AOR catalysts



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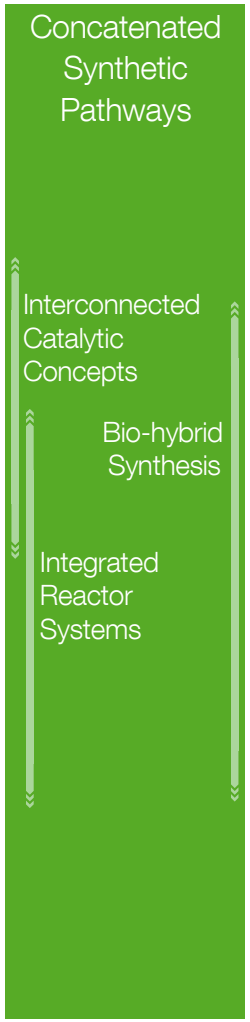
Strategic Research Area III: Concatenated Synthetic Pathways
Catalytic Toolbox to Generate a Flexible Bio-hybrid Molecular Platform



Separation Technologies

- distillation
- phase separation
- membrane
- crystallization

Catalyst & Reaction System

- activity
- selectivity
- stability
- reaction conditions

Molecular Design

- active sites
- mechanisms
- local environment

Strategic Research Area IV: Translational Catalytic Processes
Robustness and Stability despite Complex, Fluctuating Feedstocks

Translational Catalytic Processes

Feedstock Complexity & Variability

Energy Input & Fluctuation

Integrated Feedstock Supply & Conversion

Adaptive Catalytic Systems

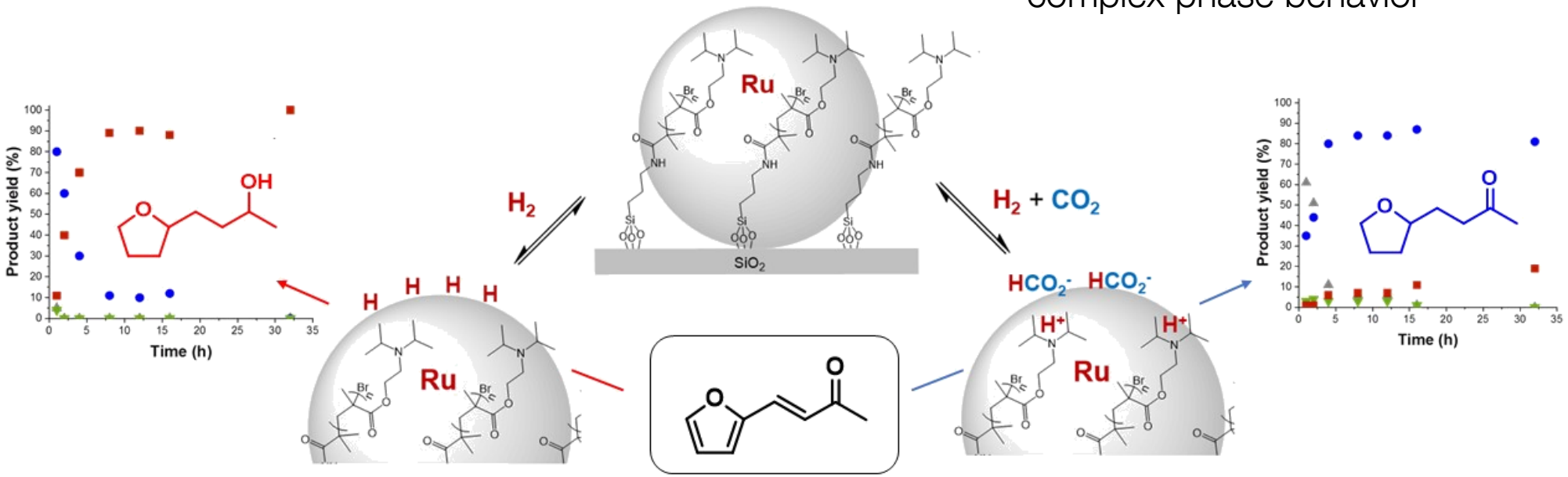
robust & flexible
phase separation
membrane crystallization

Raw Material Complexity

catalyst
transformation
reactor system

Dynamics of Catalytic Systems

operando spectroscopic techniques
online kinetic analysis
complex phase behavior



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Strategic Research Area IV: Resilient & Adaptive Conversion Systems
Resilience and Adaptivity Across Scales

Resilient & Adaptive Conversion Systems

Fuel & Chemical Design

System Integration

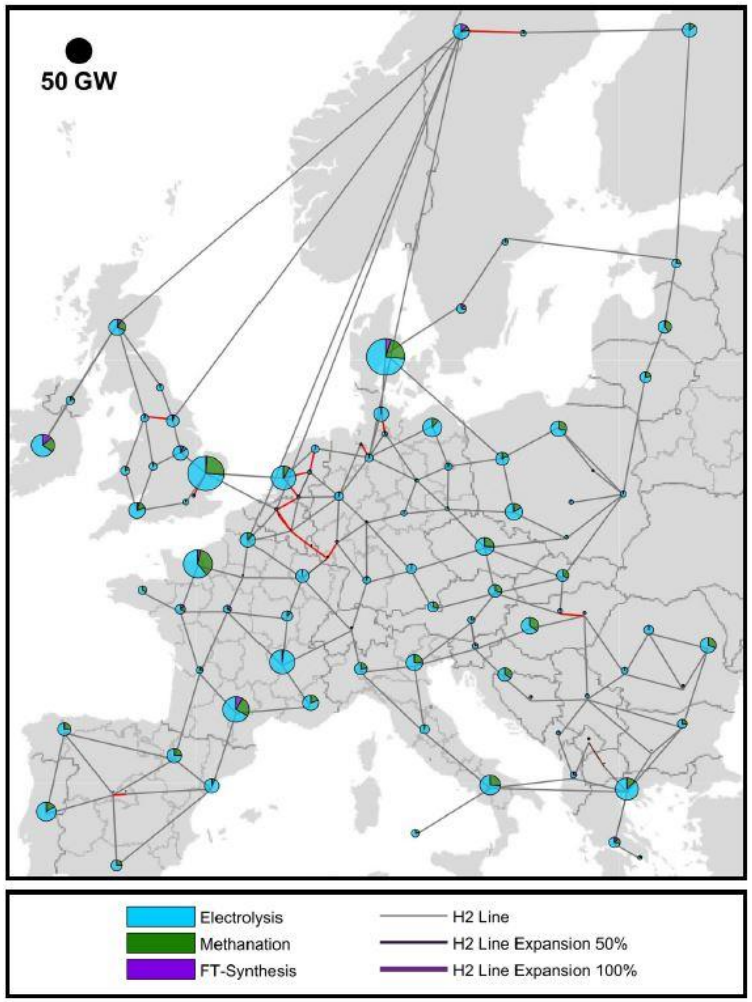
Life Cycle Assessment

Multisectoral Global Model

robust & flexible
phase separation
membrane crystallization

Holistic Sustainability Assessment

environmental
social
economical



Stakeholder Integration

stakeholders' incentives
policy design
systemic risk measures

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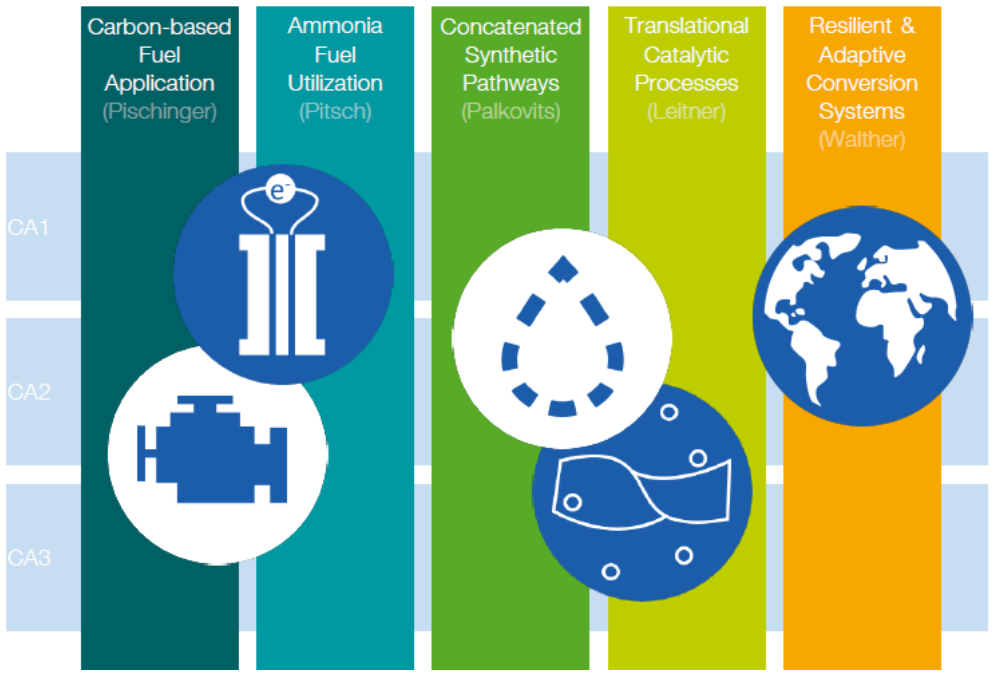
Operational Cluster Management

International Advisory Board
scientific | industrial | global | interdisciplinary

Steering Committee
representative | decisions | strategy

Cluster Office
controlling | communication | organisation

Scientific Program



Supporting Structures and Environment

Early Career Researchers (von der Aßen)
undergraduate | doctoral | post-doc | junior research group | tenure track

Equal Opportunity (Leicht-Scholten)
equity | inclusion | fairness | equality | individuality

Research Data Management (Herres-Pawlis)
interdisciplinary | FAIR | comprehensive | high quality | standardized

Quality Assurance (Pischinger & Leitner)
internal | external | independent | objective | holistic

Science Communication (Cluster-Office)
intra-cluster | public outreach | peer-reviewed | transdisciplinary