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The (Long) Way from the Basic Experiment to the Process or Material

The Profile Area “Molecular Science & Engineering” (MSE)

The scientists in the profile area “Molecular Science & Engineering” (MSE) work at the interface between natural, engineering and life sciences, combining the disciplines of chemistry, biology, physics, process engineering, mechanical engineering, and medicine (see Figure 1). The research generates basic knowledge and creates technological know-how for the design and development of molecular transformations, processes and materials. These go beyond all scales and interact to form complex and long-term adaptive systems. Thus, the profile area lays a foundation for innovation and sustainable development in a variety of application fields, with particular focus on the areas of health, nutrition, energy, and the environment.
The research projects are divided into two main areas, “Molecular Transformation” and “Soft Matter/Interactive Materials”. It is becoming increasingly clear that boundaries are blurring, and effort is needed to integrate the molecular understanding of matter transformation and material into complex processes and systems. While molecular transformation processes and the design of functional materials are focused on steady-state conditions and durable performance under optimal conditions, adaptive systems allow self-regulatory adjustment or optimization. So far, this principle can be recognized in some cases for synthetic systems only.

Biology provides the natural model for adaptive systems that self-organize at the molecular level and respond to environmental change. Biotechnology has always taken advantage of the possibility of engaging in cellular processes. Synthetic biology, as a manifestation of biotechnology, deals with the targeted engineering of molecular interaction networks in cells and cell-free systems to generate useful functionalities. Adaptive metabolic processes, molecular circuits and microcompartments play a crucial role here. Synthetic biology also represents a multidisciplinary topic between the natural and engineering sciences because technical concepts of modularization, decoupling,

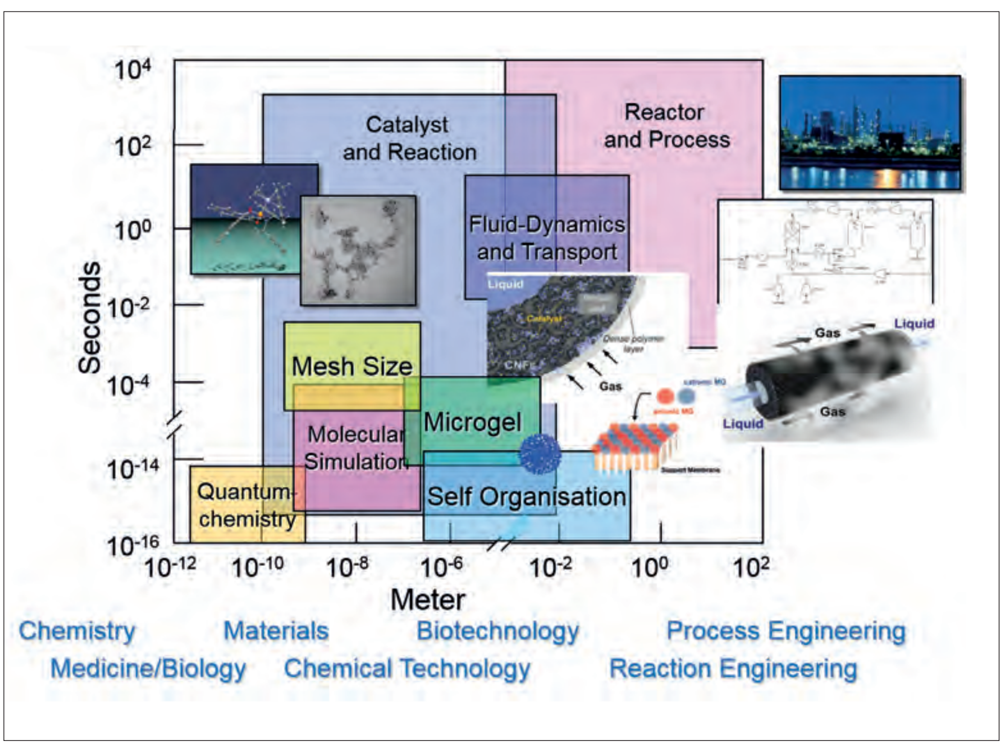

Figure 1: The cross-scale research approach within the “Molecular Science & Engineering” profile area ranges from molecular design to complex systems.

complexity reduction, automation, or computer-aided system design belong to the tools of this discipline.
The core competencies of chemistry in molecular transformation and functional materials form the basis of development. With the help of highly selective changes of the electronic and spatial structure of molecules and materials, correlations of structure or effect can be analyzed. In interdisciplinary approaches, these can be used to define inverse problems based on this structure/activity relationship. The enormous scientific and technical potential is already evident in the RWTH Cluster of Excellence "Tailor-Made Fuels from Biomass" (TMFB) as well as in the Collaborative Research Center "Functional Microgels and Microgel Systems". Furthermore, there are synergistic overlaps with the goals of the "Energy, Chemical & Process Engineering" (ECPE) profile area. It is possible to resort to complex biological materials, such as biomass, as starting materials, whose provision and adaptation are investigated across disciplines.
Only at first glance are material and reaction systems to be considered separately. The example of nature shows that the control of structure formation and compartmentalization are prerequisites for the control of complex reaction systems. In analogy, this also applies to the formation of materials. Hybrid structures also open the way to cell-free biotechnology, whose progress is ultimately impossible without an understanding of the underlying chemical processes.
Cross-scale processes already well understood in medicine can serve as models for complex synthetic systems. The variability of the form and functionality of the stimuli, including feedback mechanisms in the reaction systems, can be transferred to chemical processes and allow the conceptual replication of the "biological" functionalities of self-assembly, adaptation and self-healing into technical systems. Here, the focus is on basic medical issues in implantology and biohybrid medical systems. In addition, potential solutions are generated at the interface to the "Medical Science & Technology" profile area (MedST).
System-oriented engineering sciences benefit from the deductive analysis of materials and reactions in biology and chemistry and contribute to the understanding of molecular-level interactions, in particular structure and function as well as reaction and transport, through modeling. Cross-scale mechanistic models

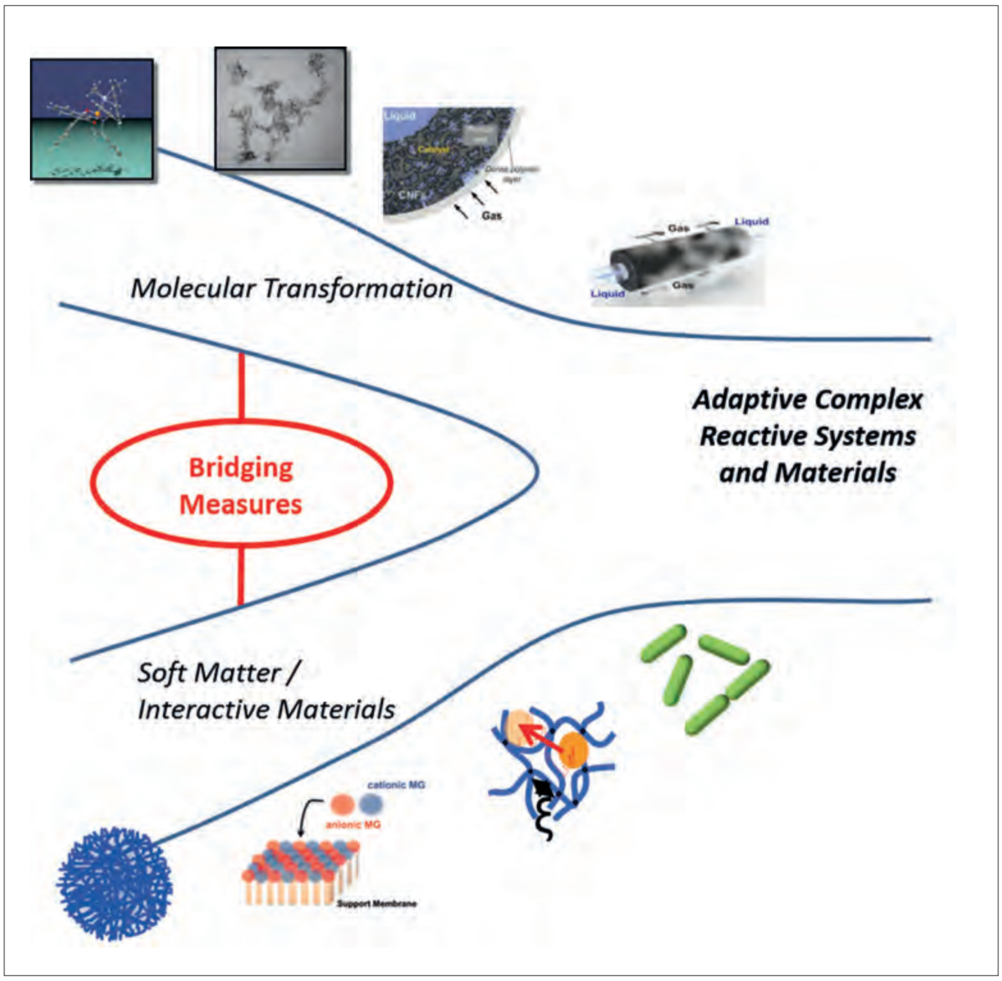

Figure 2: The merging of the two subject areas "Molecular Transformation" and "Soft Matter/Interactive Materials" with the aim of generating "Adaptive Complex Reactive Systems and Materials".

allow the formulation and solution of inverse problems and thus model identification. They are a prerequisite for the prediction of the behavior of increasingly larger structures based on molecular understanding. Based on validated models, complex systems can be designed and optimized using computer-aided design. At the same time, cellular systems characterized by compartmentalization on the sub-micron scale provide a blueprint for efficient process integration.
A quantitative understanding of the mentioned adaptive (catalytic) systems can be significantly improved by the combination of simulation and experiment. While relatively simple or small systems are accessible with ab initio simulation methods, the study of complex systems requires appropriate strategies for cross-scale modeling or an appropriate combination of model-based simulation and experimentation. The typical superimposition of reaction and transport or motion processes poses a challenge for the spatial and temporal resolution of non-invasive measurement methods. Spectroscopic methods are particularly suitable here, which, in addition to qualification, also enable quantification of (bio)chemical species. These are addressed in the FLAMENCO, RamAc and MARC competence centers.
Recent achievements and perspectives for the various interdisciplinary approaches are presented in the following contributions.

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