Small molecules

Thermodynamics, chemistry, and dynamics of small molecules/clusters/particles

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Chemical interactions, thermodynamics, and transport of compounds, clusters, and particles determine the formation and function of matter. Questions addressed range from phenomena on small length scales (single molecule experiments) or units composed of a relatively small number of particles (colloids, aerosols) to processes on larger scales such as transport in organic solar cells, through membranes, in the blood or in clouds.
The systems extend from a high level of external control to much more complex and less controlled ones (e.g. ion migration through a polymer membrane or mass transport in the atmosphere). Not only are length scales and structural aspects different, but also the sources of interaction potentials and correlation effects. A common theme of current interest throughout the whole field of the MPGC is the fact that mass fluxes, chemistry and resulting structure formation in the systems often occur far from equilibrium. Thus, a particularly high degree of synergy is expected.

Gas transport

Gas transport in materials, biology, lungs and the atmosphere

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Gas transport and system dynamics represent a theme that is of great interest to all fields participating in the MPGC. It typically occurs in heterogeneous environments, and its control is crucial for the function of artificial and natural systems alike.
This includes packaging, polymeric membranes, but also ventilation in the lung, where a large range of length scales is involved and last, but not least, the atmosphere. Gas transport in biology often involves carriers, thus it is strongly related to questions of specific binding that also are relevant in drug carriers or sensorics. Due to the low density of gases, specialized analytical tools are needed. Researchers in Mainz are world leaders in sensing transport tracers at the earth/atmosphere interface using micrometeorological techniques, in the atmosphere with specialized research aircraft (HALO), satellites, as well as MRI of the lung with hyperpolarized gases (^{3}He).

Macromolecules

Unifying characterization of synthetic and biological macromolecules and their assemblies

Source: Roland. E. Bauer et al. in Wikipedia

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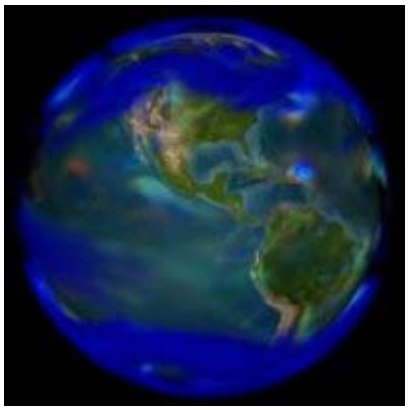
Without detailed characterization of structure and dynamics of synthetic and biological macromolecules, their behaviour and function cannot be understood and controlled. Moreover, supramolecular structures and the organization of such entities to extended functional units have to be characterized. Again, many orders of magnitude in both length and time have to be covered. Also the systems are typically not crystalline in the traditional sense.
Thus, their structure cannot be obtained with atomic resolution from conventional X-ray or neutron scattering. These techniques, however, together with electron and scanning probe microscopy are particularly powerful to obtain the structure at intermediate length scales. The combination with magnetic resonance techniques, NMR and EPR, which are well-established in the study of bio macromolecules, yields unprecedented structural information covering the whole range.
Similarly NMR and EPR yield site selective dynamics, which, when combined with neutron scattering and dielectric spectroscopy, provide new insights. The MPGC will welcome opportunities to utilize the world-wide recognized expertise in Mainz in Magnetic Resonance, Mass Spectroscopy, Optical Spectroscopy, and Electron Microscopy of synthetic systems and biological systems.

Multiscale Modelling

Multiscale modelling in materials science, biology and earth sciences



Author: Greg Shirah (NASA/GSFC)

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It is common to all these disciplines that a hierarchy of scales is addressed in order to provide a quantitative understanding of the phenomena under consideration. In earth systems modelling local and global observations have to be linked to studies of chemical reactions and kinetics under laboratory conditions.
Meteorological processes, atmosphere-biosphere interaction as well as links to the solid earth and oceans need to be understood in terms of climate control mechanisms. In soft materials science and biology, details of the local chemical structure on a molecular scale have to be linked in a systematic way to generic physical aspects, such as fluctuations and phase transitions, which can best be studied on a rather general level.
In either case, a continuous up and down scaling of the level of description is required and an improved and more profound inclusion of non-equilibrium phenomena is crucial. Groups in Mainz have contributed to this development for many years, which requires truly interdisciplinary work at the leading edge.

Bio-Atmosphere Interaction

Chemical Characterization of Biosphere Atmosphere- Interaction

Photo: Michael Welling, MPI Chemistry

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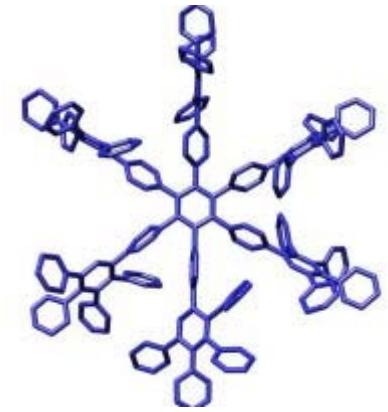
The exchange of gases and aerosols between the marine/terrestrial biosphere and the troposphere plays an important role in the chemistry of the atmosphere, influencing global climate and air quality. The quantitative understanding of these processes requires the development of sophisticated measurement techniques for atmospheric key components, their application in collaborative experimental studies (lab and field-based) and a suitable description and interpretation by modelling activities.
The fluxes of reactive nitrogen and carbon species, especially nitrogen oxides and volatile organic carbon compounds, must be determined in key environments, e.g., tropical and temperate forests. Reactions between these compounds control oxidation processes in the atmosphere and the production of organic aerosols. Both natural emissions and vegetation fires contribute to the aerosol burden of the atmosphere, which in turn affects global and regional climate, including precipitation. Long-term measurements at critical locations around the world are essential for understanding global change and for validating earth system models.

Drug Delivery

Novel Drug Delivery Technologies



Source: Wikipedia

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Polymeric systems such as polymeric nanoparticles, nanocapsules, lipsomes, hyperbranched polymers, polymer complexes and dendrimers are of increasing interest as marker systems (e.g., with superparamagnetic cores, quantum dots, or fluorescent dyes) and as drug delivery systems (consisting of biodegradable polymers like alkylcyanacrylates, poly-L-lactide, polyglycerols, or polycaprolactone and the drug) in biomedical applications.
Researchers in Mainz design novel drug delivery systems which will enable the targeted transport in biological systems. The fundamental understanding of the interaction of these new materials with cells, cellular components and proteins, and the transport into cells is only poorly studied and therefore of high interest for the MPGC.
It is the strength of the MPGC to systematically investigate the influence of nanoparticles of different sizes, materials (e.g. polarity), and functionalizations on differentiation, proliferation, and apoptosis of cells. Novel drug delivery systems established by different approaches in the will also be able to cross biological barriers such as the epithelia of the gastrointestinal tract, the lungs, or the blood-brain barrier. Stimuli-dependent responses (e.g. by changes in temperature, pH, and enzyme supply) of the drug-loaded polymeric system can lead to controlled drug release.

Complex Order

Formation of Complex Order

Photo: Rainer Sturm (Pixelio)

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In most modern materials but particularly in magnetic, in soft and in biologic matter, formation of order is not restricted to mere 1st order phase-transitions like crystallization or condensation. Rather, the focus will here be on tailored interactions between constituents and we shall exploit self organization processes under the influence of additional control fields or confinement.

Due to the competing interactions on different time and length scales, complex forms of order arise comprising a large interdisciplinary challenge. In this project we are interested in both the static aspects of order formation (phase diagrams, domain size distributions, onset of instabilities etc.) and the non-equilibrium dynamics of phase transition kinetics and relaxation processes. We thus shall cover extended length and time scales from the microscopic to the macroscopic regime as well as from ultrafast processes to slow relaxations.

Examples of interest for this group include twin pattern formation in shape memory materials coupled to magnetic order, soliton stair cases evolving to standing strain density waves in thin metal films or confined colloidal crystals, hierarchical order by different effective interactions on different length scales in colloidal or biological materials or multi scale dynamics of magnetic phase transitions.

This program unites materials chemistry with biology and colloid physics in state of the art system design and experimental characterization. It will expand to include the designated

successors of F. Schmid & Prof. Adrian and should be supported by an experimental W2-position supplementing the existing expertise on optical techniques and spectroscopy with fast scattering methods. This position would also be of great importance for the research topic of novel organic charge transfer salts and further research on fast structural or magnetic processes throughout the MPGC.

Theory and simulation on the other side integrate the different material classes by suitable conceptual work & multi scale simulations. Hence, this connects the present research topic to the corresponding research topic, where the techniques of multi-scale simulations are developed. Progress in this topic, of course, will immediately affect also other subjects and thus provides strategic support to the centre.

Bio Atmosphere Processes

Biological processes interacting with the Atmosphere

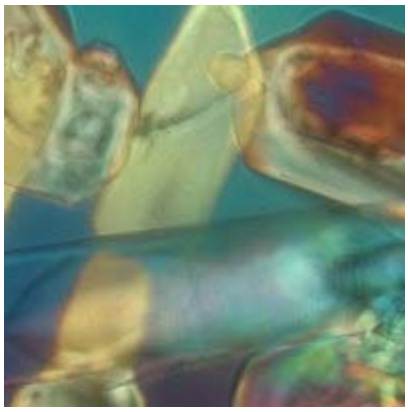

Photo : Dr. Karl Herrmann (Pixelio)

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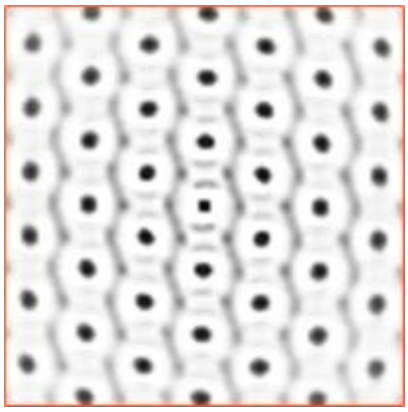
Understanding the interactions between biosphere and the atmosphere is a key for our understanding of atmospheric chemistry and physics and for the evaluation of earth system models. Biological contributions by higher vegetation, soil biology, algae, cyanobacteria, lichens and mosses significantly affect the exchange of trace compounds between the earth surface and the atmosphere.

Similarly, consumption of anthropogenic trace compounds contributes to these aspects. All these processes have a significant influence on local, regional and global climate. This way, climate research is closely related to the fields of botany, plant physiology, phycology and microbiology coupling exchange studies with physiological/biochemical processes, such as photosynthesis, respiration, transpiration and enzymology. Investigations of the exchange of stable as well as reactive trace gases between soil/vegetation and the atmosphere cover scales from the enzymatic processes up to regional flux measurements and satellite observations.

Compounds of interest for example are Non Methane Hydrocarbons (NMHC) or Volatile Organic Compounds (VOC, Monoterpenes, isoprene, oxygenated compounds, acids, aldehydes) as well as reduced sulphur compounds (H_2S, COS, CH_3SH, DMS, CS_2). The spectrum of compounds involved and the complex interactions in nature needs a close cooperation between several research disciplines such as biology, chemistry and physics merging the scientific as well as analytical questions.

Complex fluids

Complex fluids in restricted geometry



Source: Ralf Biehl FZ Jülich

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When mesoscale particles like macromolecules, drug-carriers, fibres or colloidal spheres are immersed in a carrier fluid, a so-called complex fluid emerges which displays fascinating mechanical and optical properties not seen in the constituents. In particular, suspensions of colloidal spheres or rods form fluid or (liquid-)crystalline ordered states once the range and strength of interaction between the colloidal particles becomes sufficiently large and long-ranged. Their equilibrium properties are meanwhile quite well understood. However, without a decent understanding also of the non-equilibrium properties and the influence of confinement to small system sizes, no controlled application will become possible. Questiones touched here comprise freezing and melting in small pores, yielding of materials under strong load, shear induced ordering or microfluidic transport of drug carriers. The MPGC joins experimental and theoretical expertise to address such problems by complementary approaches from theory, simulation and experiment.
The interplay of long-range hydrodynamic and electrostatic interactions with confinement effects leads to a wealth of intriguing phenomena which are a challenge to simulation approaches. The MPGC provides an excellent environment for the development of new efficient methods to solve this problem and their application e.g. to electrophoresis and dielectrophoresis. The making and manipulation of structures with defined optical properties on the other side is subject of experimental studies employing shear, electric fields and restricting geometry, e.g. systems confined in narrow slits or capillaries.
The intense collaboration and exchange between the complementary approaches within this Centre provides a fertile ground for advancing our understanding and control of the fundamental physics governing the fascinating properties of complex fluids.