Call for Proposals

No. 40 **13 July 2020**

Priority Programme "Creation of Synergies in Tailor-made Mixtures of Heterogeneous Powders: Hetero Aggregations of Particulate Systems and Their Properties" (SPP 2289)

In May 2020, the Senate of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) established the Priority Programme "Creation of Synergies in Tailor-made Mixtures of Heterogeneous Powders: Hetero Aggregations of Particulate Systems and Their Properties" (SPP 2289). The programme is designed to run for six years.The present call invites proposals for the first three-year funding period (starting app. in mid. 2021).

Mixing of disperse systems (particles and powders) is a traditional unit operation of process engineering which is of central importance in various technological areas. Applications of mixed particulate systems range from processing of food, pharmaceutical and chemical substances to material processing and materials engineering. Functional mixing of different particle types (hetero-aggregation) has the potential of creating outstanding new properties of dispersed products, which depend on the mixture composition (e.g. number of components, concentration, total quantity) and on various secondary process conditions (e.g. agglomeration, coating).

In this context, a new product property can emerge from the direct contact of different particles (hetero-contact) and thus by the resulting interface between the respective particular components. Many applications have shown that these hetero-contacts are of fundamental importance for specific functional properties. In most cases the new properties result from the transfer of charges, mass, heat, forces, or moments without the need of a chemical reaction of its components. Thus, the quality of such a particulate mixture is directly linked to the contact points and interfaces of different particles and the details of the interaction between its species in contact.

The new property from the contact zone controls the material and product properties of the entire system that is named hetero-contact in the context of the Priority Programme. Direct information about hetero-contact quality (e.g. number of contacts, transport properties between different particle types) could therefore be the base for a fundamental description of the new properties of the particle mixture (quality of the mixture and material function). At the same time, the hetero-aggregation process for creating of such hetero-contacts needs to be investigated and controlled.

The technical main goals and development areas of the Priority Programme therefore are

- the development of sophisticated methods for the characterisation of hetero-aggregates in disperse systems,
- the development of suitable process diagnostics that feature component-specific detection,

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- the derivation of proper process descriptions and simulations with validated models (particle, continuum and/or population based) for mixtures of < 1 µm sized particle systems, and
- the establishment of efficient model couplings (e.g. DEM-CFD) for the ab-initio gas phase process design.

These goals aim to a fundamental understanding of the relevant mixing phenomena on length scales in the sub-micrometre range and their modelling as well as transfer into applications of tailored hetero-aggregated particulate systems and aggregation processes.

The processes for designing hetero-aggregates are divided into the formulation (from existing particle systems) and the production (from molecules and their reaction products) of the hetero-aggregates. The solely focus of the programme is on processes in the gas phase, where both adhesion forces and specific charge distributions of particles play an important role. Gas-phase aggregation processes can be implemented with different methods and reactor concepts. The advantage of direct mixing in the gas phase is the prevention of undesired phases, the adjustment of any mixing ratio, the definition of the particles (size, crystallinity, phase purity, shape etc.) independent of the mixing process itself and the deliberate creation of a new property by the newly created interface. The specific challenges for these systems and processes arise especially for particles smaller than 10 µm in size and cover a broad size range over three decades down to 10 nm. In this size range, mass inertia forces are almost negligible compared to adhesion forces and particle transport is dominated by diffusion. Here, the mixing process is to be determined with respect to the relevant turbulent multiphase flow scales.

The synthesis of hetero-contacts can be achieved by mixing existing particle systems (A+B) (formulation) and/or by a sequential production process, which often involves nucleation of the second phase on top of the first (B on A) (production). In any case, the initial particle properties of all disperse phases (hetero-phases) involved in the process must be prescribed and formulated with a specific view onto the subsequent contacting process and the targeted remaining contact quality. In addition to the chemical composition of the particles, the particle shape and the surface morphology of the particles are particularly of interest during particulate processing.

In the first three years of the Priority Programme the recursive approach is dominant, in which the material system of the hetero-aggregates is adapted to the process measurement technology and the characterisation procedures of hetero-aggregates and their populations. Specific emphases are:

- on the establishment of aerosol processes for the defined generation of hetero-aggregates, which can also be adapted to process diagnostics for the detection of mixing processes < 1 µm,
- the derivation of particulate sampling trains from fast aggregation processes,
- the establishment of tomographic methods for the characterisation of hetero aggregates with sizes < 1 µm, and
- their mathematical framework for the description of hetero-aggregates as well as
- the establishment of process models and simulations covering mixture lengths < 1 µm.

Here, proofs of principal material functions are to be predefined or described from the established hetero-aggregated particulate systems.

For the strategic long-term goals, the Priority Programme in the second period and finally after six years is directed towards:

- developments of in-situ process and particle analysis tools with time scales of a few milliseconds and length scales below one micrometre (< 1 µm),
- tailoring material properties and functions of hetero-contacted particulate systems,
- transfer of new products of hetero-aggregated material systems into application.

The Priority Programme is subdivided in four research focus areas:

- preparation and formulation of hetero-aggregates
- process measurement technology for hetero mixing processes
- modelling and simulation of hetero mixing processes
- characterisation of hetero contacts and aggregates and their material function

In order to ensure synergetic processes and focus the measuring techniques the programme considers only mixing processes in the gas phase. At the same time, the projects are expected to cover at least two of the above-mentioned thematic blocks comprehensively. All projects must consider the quantification of the mixing quality / mixing processes with respect to the hetero-contact. Individual project proposals that address a strong interlink with other projects within the programme are appreciated. In order to foster the cooperation of projects already in their design phase, applicants are encouraged to submit their intended topic and contact details on a login-secured website (once the applicant topic is listed, the topic and details of others can be seen). Login details are available after sending the details to the coordinator by e-mail.

The Priority Programme does not consider mixing processes in the liquid phase, observation of nucleation processes without particulate systems, consideration of isolated individual processes without integration into the overall concept and analyses of particulate structures in the size range larger than 10 µm.

Proposals must be written in English and submitted to the DFG by **10 November 2020.** Please note that proposals can only be submitted via elan, the DFG's electronic proposal processing system. To enter a new project within the existing Priority Programme, go to Proposal Submission – New Project/Draft Proposal – Priority Programmes and select "SPP 2289" from the current list of calls.

In preparing your proposal, please review the programme guidelines (form 50.05, section B) and follow the proposal preparation instructions (form 54.01). These forms can either be downloaded from our website, the SPP website (www.spp2289-heteroaggregates.de) or accessed through the elan portal.

Applicants must be registered in elan prior to submitting a proposal to the DFG. If you have not yet registered, please note that you must do so by **27 October 2020** to submit a proposal under this call; registration requests received after this time cannot be considered. You will normally receive confirmation of your registration by the next working day. Note that you will be asked to select the appropriate Priority Programme call during both the registration and the proposal process.

The proposals reviewing process will include a colloquium with direct presentations and discussions of applicants and reviewers, planned in March 2021. The date and location of the colloquium, as well as all other relevant updates, will be published on the homepage of the Priority Programme in due course.

Further Information

More information on the Priority Programme is available under:
www.spp2289-heteroaggregates.de

The elan system can be accessed at:
https://elan.dfg.de/en

DFG forms 50.05 and 54.01 can be downloaded at:
www.dfg.de/formulare/50_05
www.dfg.de/formulare/54_01

For scientific enquiries please contact the Priority Programme coordinator:
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