Engineered nanomaterials (ENM) constitute the core of numerous advanced technologies. Nevertheless, next to the indisputable advantages related to the unique ENM features, the increasing environmental release of ENM and consequently, the increasing exposure and potential adverse effects on human health and environmental safety should be considered. Reliable risk assessment includes exposure assessment (in addition to hazard assessment). However, a comprehensive experimental research is unfeasible due to the vastness of nano-forms diversity in terms of their chemical and physical differentiation. Nonetheless, the fundamental issue is getting to understand transformations mechanisms of ENM in environmental conditions, their transport and environmental fate. Here, the exploitation of sophisticated chemoinformatic methods may become valuable in recognition of significant dependences between pristine nano-form of ENM and properties in environmental conditions, based solely on partial, available experimental data.

FateNANO is aimed at addressing the question: Which structural features of ENM nanoforms are responsible for determining their release, environmental transport and fate and thus human and environmental exposure?

The crucial parameters determining environmental ENM transformations and fate such as dissolution and agglomeration will be identified by developing a quantitative nanostructure-property relationship (nano-QSPR) modeling, which will permit to link structural features of the primary ENM with their properties after environmental transformations. In order to identify the nanoforms released to the environment from nano-products, a form-specific release model based on material flow analysis (MFA) will be developed. This new model will also incorporate the particle size distribution of the released ENM. The complete information provided by the new release model will enable a full coupling of MFA and environmental fate modeling (EFM), for which information on the particle form and size distribution is crucial input for predicting environmental fate of ENM.

The accomplished knowledge and the developed hybrid nano-QSPR-MFA/EFM methodology will make possible the estimation of environmental exposure of new nanomaterials based solely on the initial structural features of pristine ENM and before their release into the environment. Therefore, the output of the project will be the delivery of the complementary knowledge and methodology next to the hazard assessment in the overall risk assessment of nanomaterials. The proposed computational approach for estimation of environmental transformations, transport and fate is in line with the safe-by-design strategy for developing new, safer materials through predicting potentially adverse properties for human health and environmental safety at the design stage and without the necessity of extensive, costly and time-consuming experimental research.