Systematic machine-learning (ML) supported investigation of the design space for nanoparticle syntheses with the aim of creating organic-inorganic hybrid systems

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The development of photoinitiators is an important and challenging topic due to the many applications, as they are used both on an industrial scale and for consumer (3D printing). The advent of new light sources (LED, LCD) has further increased the demand for new photoinitiators. As the various photoinitiators are highly reactive chemicals, they must also be evaluated in terms of their risk to human health relative to their benefit. In particular, bulk free radical polymerization and interaction with photoinitiators and other compounds in resin blends is a difficult subject that is very complex, especially with regard to interaction with the atmosphere (oxygen). From a practical point of view, migration, which can be defined as any process leading to possible contamination by photoinitiators, such as diffusion or gas phase transport (e.g. into the interior of food packaging), is of crucial importance. We have tested and discovered different types of photoinitiators where the chromophore is based on an inorganic particle. These photosemiconductors are low-migration or migration-free initiators because their size prevents them from diffusing or evaporating. The prototype of a ZnO-based fragmentation PI works well in the UV-A range. A number of challenges have been identified, but we are particularly interested in the first stage, namely the formation/control of nanoparticles and their modification (basic research for a more stable foundation).

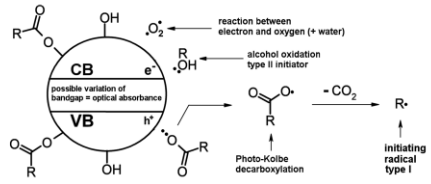
- Understand the improvement of precipitation conditions for ZnO based systems with the A|S (ML) process. (output: Crystallinity, size, aggregation, surface charge, dispersion quality aspects in different resins, see below)
  → Large number of experiments will be necessary

HERE, we will apply the developed A|S method for multidimensional ML analysis to analyse the design space and identify influencing factors in order to improve the robustness of the synthesis, among other things.

- Transfer and testing of ML methods on various (yet to be defined) particle preparations.

With regard to the organic-inorganic hybrid system, the focus is on modification (maintain the status quo), so the following is only touched upon:

- Investigation of the relationships between surface modification and quality in various resin mixtures (‘storage time’, dispersion quality) in combination with photoinduced radical polymerisation with regard to yes/no. (This project is considered the basis for a stable foundation = basic research.)



Scheme 1 : ZnO-light induced fragmentation of surface attached groups leading to radicals.

[1] **M. Schmitt**, Nanoscale, 7, 9532-9544 (2015).