Machine learning based artificial simulation to evaluate the synthesis and reactivity of particle based fillers

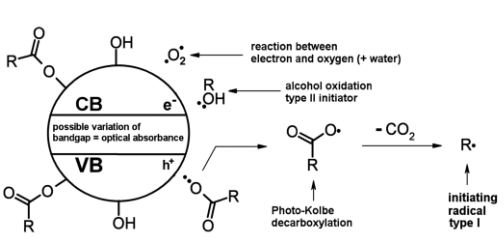
DIRECTEUR DE THESE : MICHAEL SCHMITT
CO-ENCADRANT : FABRICE MORLET-SAVARY
INSTITUT DE SCIENCE DES MATERIAUX DE MULHOUSE (IS2M) CNRS UMR 7361 UHA, 15 RUE JEAN STARCKY, 68057 MULHOUSE CEDEX
TEL : 03 89 33 88 06 ; E-MAIL : Michael.Schmitt@uha.fr

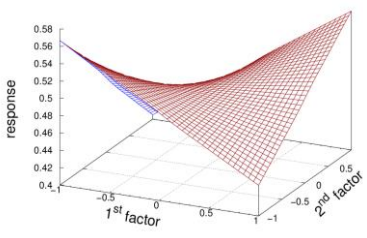
These days, the terms 'digital transformation', 'industry 4.0', 'machine learning' and 'artificial intelligence' are commonplace. To demonstrate the problematic nature of the situation, I'd like to quote a coating company expert (Ulf Stalmach (Orontec, 2021)): 'jeder spricht drüber, aber gesehen hat's noch niemand. ('everyone talks about it, but no one has seen it yet...'). A Artificial intelligence undeniably has great potential if large data sets can be trained (as is the case for languages). The proposed project crosses the boundaries of data science, chemistry and materials science. We try to develop a stochastic design of experiments (DoE) based on machine learning, called 'artificial simulation', the naming is emphasise the goal of obtaining/simulating effect diagrams (patterns). We plan to improve and understand the development of nanoparticle synthesis, to use as fillers and photocatalysis, among others. M. Schmitt discovered a prototype ZnO-based fragmentation photo initiator[1] working well in the UV-A region. Even a first study addressing the red shift of adsorption has been published in a communication. A number of challenges have been identified that can be addressed using a stochastic DoE in a scientific study:

- Understand the improvement of synthesis conditions for differnent Nanoparticles (ZnO, $FeFe_2O_4$, …) with the AS **process**. Output parameters can be crystallinity, size, aggregation, surface charge, dispersion quality aspects in different resins.
    - Modification of the band gab e.g. using Na_2S hydrate for ZnO

Data processing with the AS method makes it possible to analyse several results simultaneously, so that the process of analysis can be supplemented by application and testing of the material in polymer matrices

- Testing the understanding of the relationships between surface modification and quality in different resin blends (overlapping "storage" time relationships). Output like hiding power of different dispersions, sedimentation stability could also be included.
- Testing the reactive properties of the photosemiconductors used as photoinitiators in monomers or as photocatalysts in polymers (also recycling aspects) and the influence of the particles on the mechanical properties.





Scheme 1 : ZnO-light induced fragmentation of surface attached groups leading to radicals. Response surface computed using AS method.

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