Chemoinformatics Methods for Supporting Sustainability-By-Design Strategies

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The idea sustainability-by-design brings together the concerns of developing new materials that are at the same time effective in their applications, safe for human and "green".

Considering that there are thousands of combinations of structural features driving physical-chemical properties, behavior and toxicity of advanced materials, it is impossible to empirically test all of them. On the other hand, without having the appropriate testing strategy, the selection of objects to be studied is often made by chance and not guarantee that the finally selected 'lead material' possesses the highest possible effectiveness and the lowest hazard. For this reason, the development and application of sustainability-by-design strategies that combine experimental work and chemoinformatics methods seems to be a promising solution resulting in significant reduction of time, costs and – in parallel – the increase of efficiency and safety.

In this presentation, the idea of sustainability-by-design in the context of developing advanced materials will be briefly discussed. Then, the available chemoinformatic methods will be reviewed together with providing several examples of the successful predictions of both physical-chemical properties and a variety of toxicity endpoints. Finally, the idea of using chemoinformatics in sustainability-by-design will be deliberated.